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THE PARTIAL OXIDATION OF n-BUTANE IN HOMOGENEOUS
AND TRANSPORTED BED REACTORS

BY



MD. JASIMUZZAMAN

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES
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DEPARTMENT OF CHEMICAL AND PETROLEUM ENGINEERING

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled THE PARTIAL OXIDATION OF n-BUTANE IN HOMOGENEOUS AND TRANSPORTED BED REACTORS submitted by MD. JASIMUZZAMAN in partial fulfilment of the requirements for the degree of Doctor of Philosophy.

ABSTRACT

Experimental investigations of the partial oxidation of n-butane with air were carried out in homogeneous and transported bed reactors. The effects of the inlet temperature and the inlet hydrocarbon to oxygen ratio were studied in the homogeneous reactor. The inlet temperature affected the induction period, but the overall distribution of the products remained relatively unaltered. The hydrocarbon to oxygen ratio affected the temperature rise and the product selectivity, higher ratios leading to lower temperature rise and better selectivity in the reactor.

Simplified kinetic schemes were proposed to describe the reaction and the parameters of two such models were estimated by a numerical method using the data for conversion and temperature. The two models were tested using them to predict the temperature profiles and conversions for a number of independent runs made earlier in this laboratory.

Solid particles in a transported bed reactor take up the heat of reaction and reduce the temperature rise in the reactor. Solution of a theoretical model for a transported bed reactor revealed that the radial variation in temperature of solid particles 50 to 800 microns in diameter is insignificant. The homogeneous reactor used in the present study was provided with solids feed, heating and separation systems in order that it can be used as a transported bed reactor. Experimental runs were carried out in this reactor in a relatively narrow range of solids to gas loading ratios between 3 and 5. The selectivities to different products were compared to those in the homogeneous reactor. A significant increase in the selectivity to

oxygenated products was achieved. For runs carried out under similar conditions, the selectivity to oxygenated products rose from 0.30 in the homogeneous reactor to 0.50 lb-mole/lb-mole n-butane reacted in the transported bed reactor. For the range of operating conditions in the present study, no effect of surface was observed and the kinetic models proposed for the homogeneous reactor could be used to predict the overall conversions and temperature profiles in the transported bed reactor.

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CHAPTER I

INTRODUCTION

The slow gas phase partial oxidation of hydrocarbons takes place by degenerate chain branching and results in the formation of a large number of products such as olefins, alcohols, aldehydes, ketones, and lower paraffins. The reaction is often an economic route for the production of the oxygenated compounds. Since these products are more expensive than the parent hydrocarbons, there is an economic incentive for the process. The reaction has also been used in recent years to obtain unsaturates from the paraffins.

A large volume of work on the partial oxidation reactions has been reported in the literature over the past seventy years. However, the complexity of the reaction has frustrated efforts at establishing a mechanism for the reaction, and contradictory results are reported on the effects of different variables. The selectivity of the reaction is poor and though the economy of an industrial process must depend on improved selectivity, published information on this aspect is scarce.

An important variable in hydrocarbon oxidation is the temperature of the reaction system. In an adiabatic plug flow reactor, the reaction starts with an induction period followed by a very rapid rise in the reaction rate and in the temperature of the reacting stream, due to the evolution of a large amount of heat. This rise in temperature causes a decrease in selectivity by changing the course of the reaction and/or by further oxidation of the desirable components at the elevated temperatures.

In a transported bed reactor, inert solid particles are carried with the gas to take up the heat of reaction and hence control the rise in temperature. By a suitable choice of variables, it is likely to be possible to obtain an almost isothermal operation, or even to obtain a prescribed optimum temperature profile in the reactor. This would improve the selectivity and hence the economy of the process.

A number of studies have been carried out in the University of Alberta on the partial oxidation of n-butane in the last two decades. More recently, in 1966, Anderson (1) built a reactor with multiple sampling points and temperature probes along the length of the reactor. This reactor was modified in the present investigation to operate both as a homogeneous reactor and as a transported bed reactor. Experimental investigations were carried out in the homogeneous reactor to study the effect of inlet temperatures and inlet n-butane to oxygen ratios on the overall oxidation process and on the product distribution.

Selectivity in the transported bed was investigated and compared with the results from homogeneous runs. Mathematical models for the reactors were formulated based on the postulation of certain kinetic schemes for the reaction.

CHAPTER II

LITERATURE REVIEW

2.1 INTRODUCTION

The main research interest in the partial oxidation of hydrocarbons is due to its industrial importance. In chemical industries, a wide variety of hydrocarbons from petroleum stock are allowed to undergo incomplete combustion, leading to the derivation of all kinds of intermediate products in heavy organic synthesis. The choice of optimum conditions for the partial combustion process is very important, since both the yield of the valuable products and the capital investment for the industrial application of the process depend on this choice.

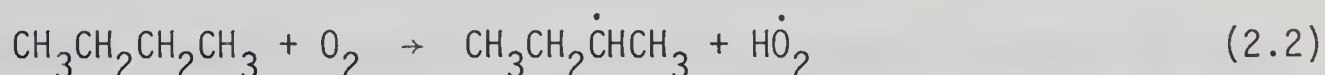
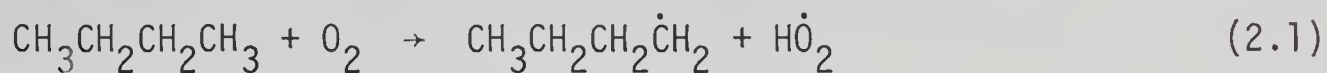
The knowledge of the mechanism of the reaction would make the choice relatively easy, but the mechanism is very complex and is not yet known. Hence, research in hydrocarbon oxidation almost always had two objectives in view: to elucidate the mechanism of the reaction and to search for the optimum reaction conditions. In the following sections, present status of knowledge in these two areas is reviewed.

2.2 MECHANISM

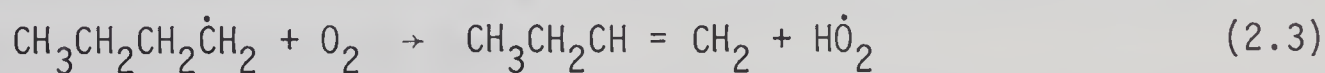
The vapour phase partial oxidation of paraffins is a free radical reaction with degenerate chain branching. The basic experimental facts concerning the hydrocarbon oxidation are relatively well established. However, the detailed nature of the complicated series and parallel steps leading to the formation of a host of intermediate and end products is far from being understood.

The initiation reaction is today almost universally accepted to be a reaction between a paraffin (shown henceforth as n-butane) and an

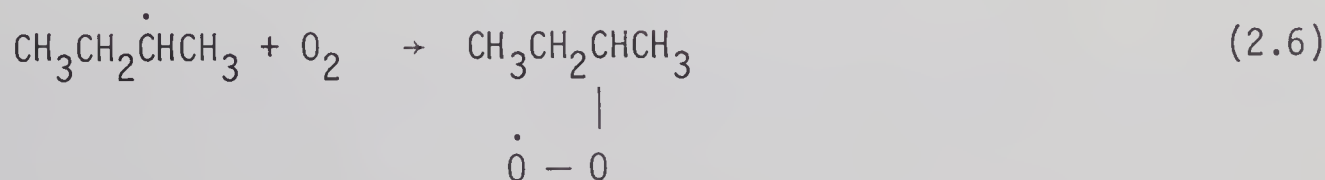
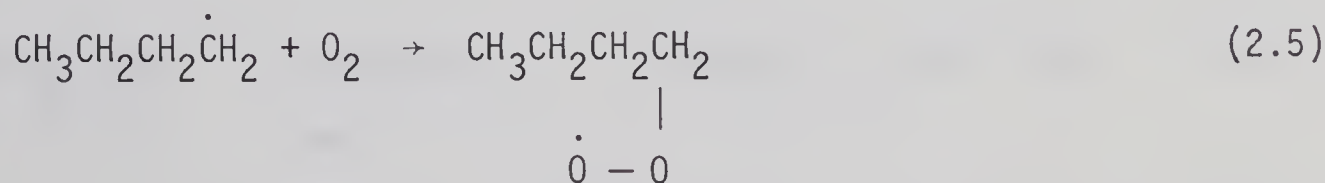
oxygen molecule⁽²⁾. The reaction normally takes place in the gas phase with an activation energy of 40-50 kcal/mole and with an equal amount of endothermic heat of reaction. This initiation leads to the formation of a butyl radical and a hydroperoxy radical. The C-H bond in the CH₂ group of n-butane is 2-3 kcal less than that in the CH₃ group and hence the amount of iso-butyl radical formed will be larger than the n-butyl radical. This effect will be more pronounced at lower temperatures, when a small difference in the activation energy can direct the course of the reaction.



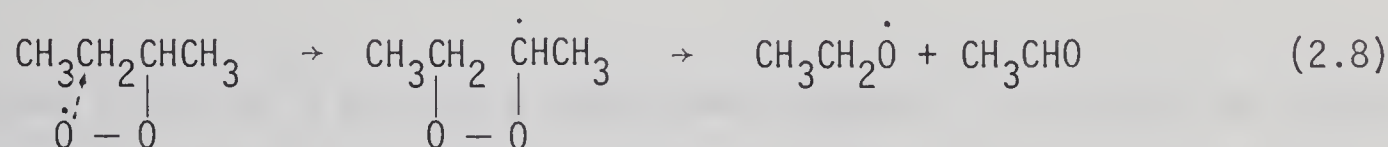
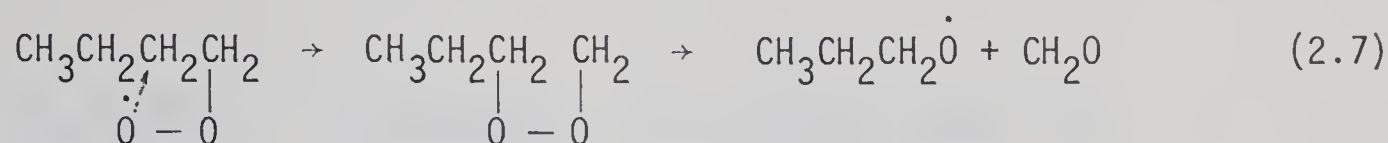
The initiation reaction is followed by a complex series of propagating steps. The butyl radical formed can react either with an oxygen molecule forming olefin as proposed for propane by Lewis and von Elbe⁽⁴⁾ and later supported by several authors^(5,6):



or it can combine with oxygen forming a butyl peroxide radical as suggested, among others, by Hinshelwood⁽⁷⁾.

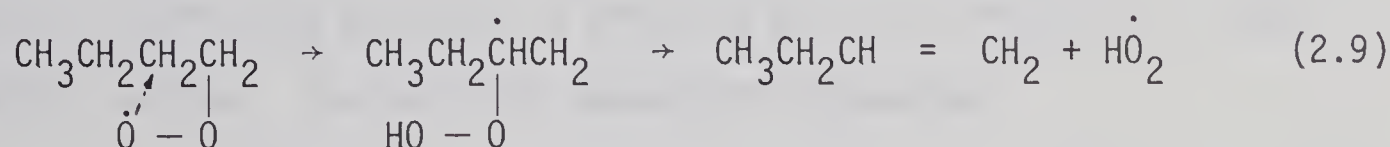


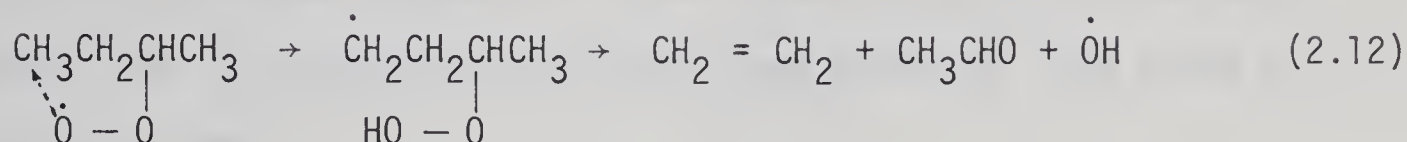
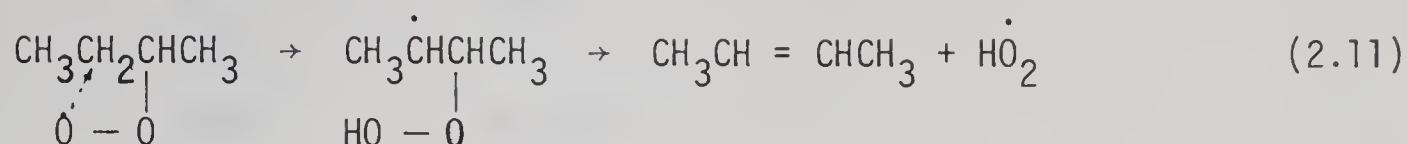
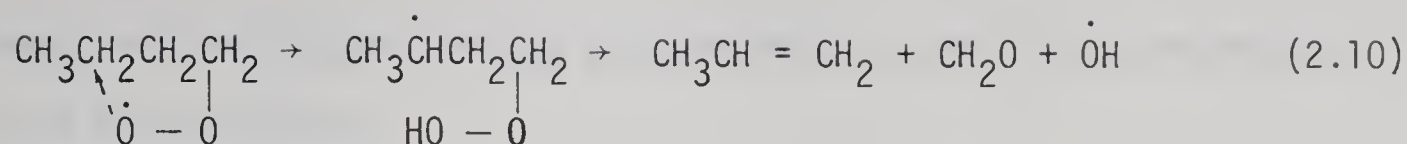
Semenov ^(2,3) and Shtern ⁽⁸⁾ developed a mechanism based on the isomerization of the peroxy radicals formed as above. The oxygen atom bearing the free valence of the peroxide radical can attack a C-C bond in the radical itself leading to isomerization and subsequent decomposition:



This method of isomerization first proposed by Shtern involves the rupture of a C-C bond and the formation of a C-O bond, and is thermoneutral. The second step, the break up of the isomerized radical is exothermic since a C = O bond (75 kcal) is made at the expense of an O-O bond (40 - 50 kcal). The activation energy of this step is probably low and isomerization is the rate determining step. Semenov obtained a value of 20 kcal/mole for the activation energy.

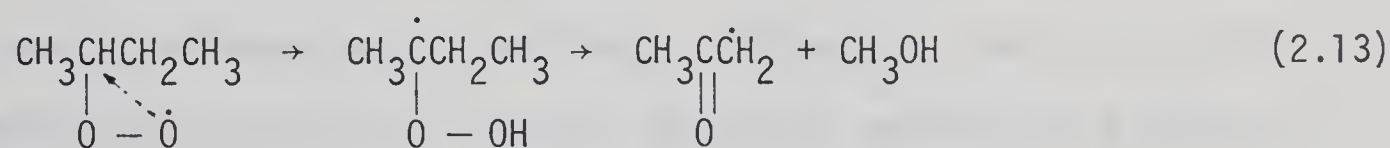
Another type of isomerization suggested by Semenov is the migration of a hydrogen atom from the carbon atom to the oxygen atom, with rupture of a C-H bond (95 kcal) and formation of an O-H bond (103 kcal), followed by decomposition.



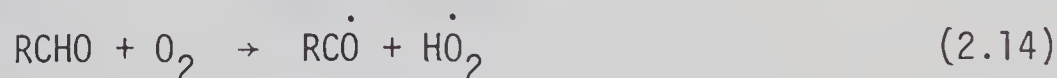


Reaction (2.12) will be highly endothermic because it involves the rupture of a C-O bond (75 kcal) and formation of a C=C bond (57 kcal) and a C=O bond (75 kcal). Isomerization will again be the rate determining step and the activation energy in this case has been calculated to be higher than in isomerization with attack on C-C bond.

In addition to this, there can be an isomerization involving the rupture of both the C-C bond (75 kcal) and the C-H bond (95 kcal) with the formation of a C-O bond (75 kcal) and an O-H bond (103 kcal).

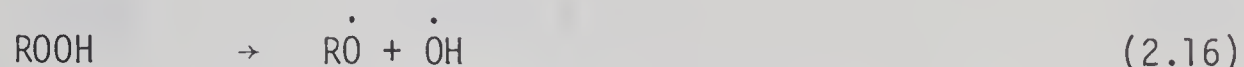


A large number of further reactions of the intermediates and the free radicals follow. But meanwhile, the number of radicals in the reacting system must multiply in order to give the reaction its autocatalytic nature. Two possible routes are suggested:



Alternatively, the alkyl peroxy radical formed by reactions (2.5) and (2.6)

can react with an alkane forming a hydroperoxide, which can decompose into two free radicals:

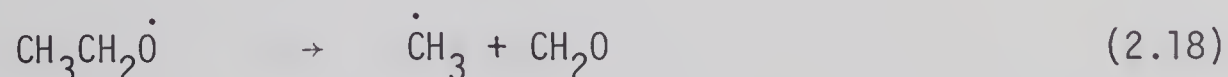
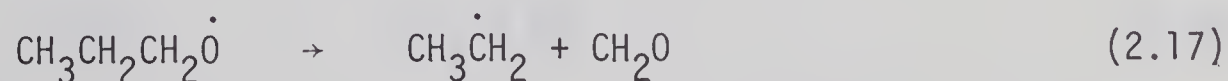


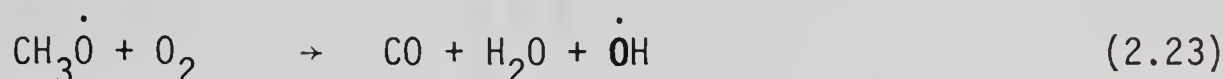
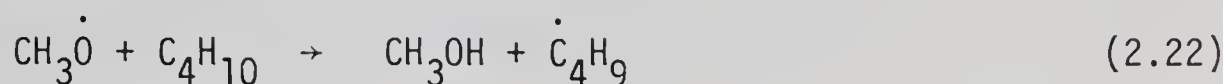
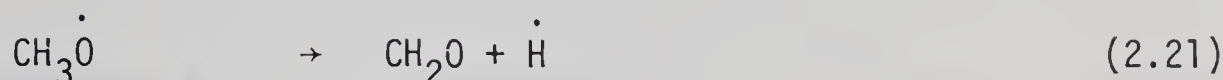
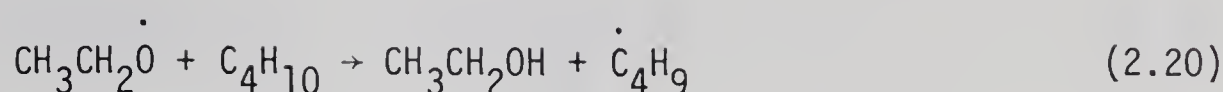
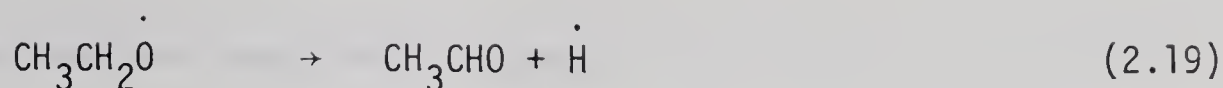
Experimental evidence for each of these branching processes has been advanced, but it is possible that both these processes take place in a reaction system.

Each of the branching process results in a net increase of two free radicals. The reaction thus starts slowly with an induction period during which time only small amounts of the paraffin and oxygen react. Finally, sufficiently high amounts of branching agents are obtained leading to the formation of a large amount of free radicals and resulting in a rapid rise in the rate of the reaction. The reaction is highly exothermic and in an adiabatic reactor, the rise in rate is accompanied by a sharp rise in temperature of the reacting mixture.

The number of free radicals in the system eventually drops to zero because of termination reactions. The termination can occur by recombination of radicals, reaction leading to nonreactive products, or by contact with the surface.

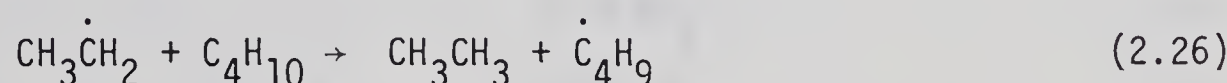
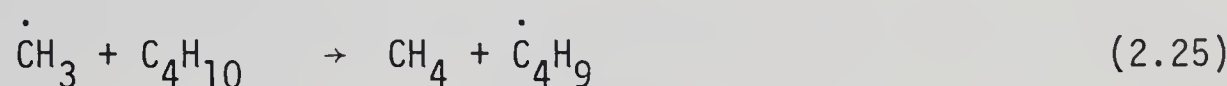
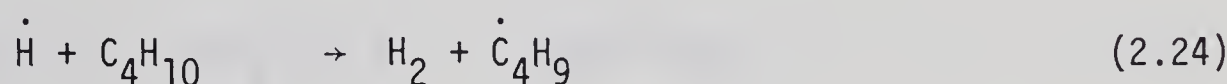
The different radicals formed in the system can react in a variety of ways. The alkoxy radicals formed can decompose or react with oxygen or hydrocarbon molecules as follows:



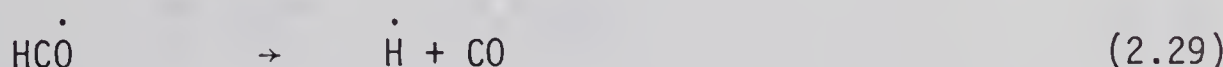
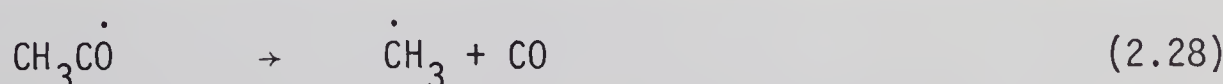
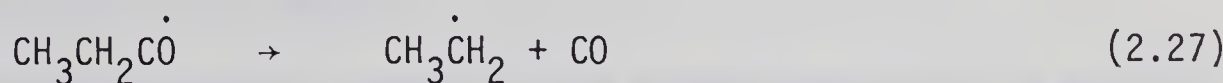


For alkoxy radicals higher than the methoxy radicals, the decomposition reaction is likely to predominate.

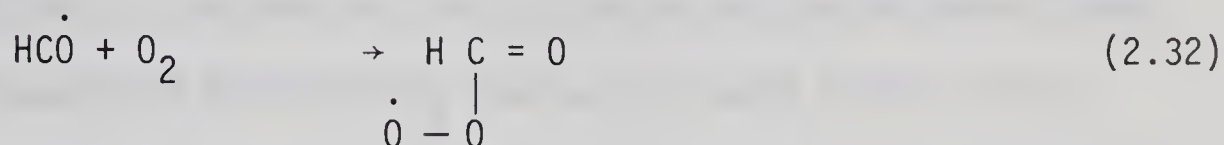
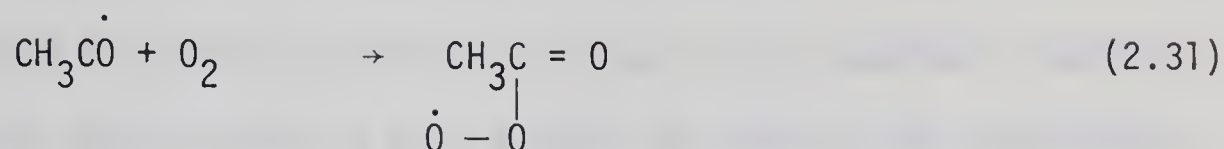
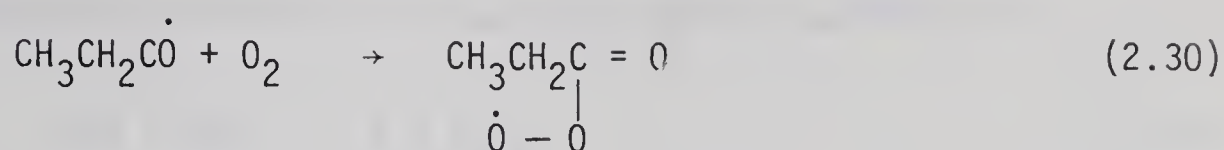
The lower alkyl radicals formed can react with an alkane molecule forming the lower paraffins. The hydrogen radical also can react in a similar fashion.



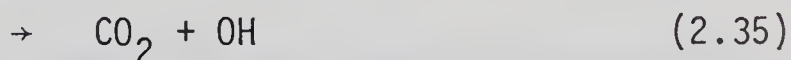
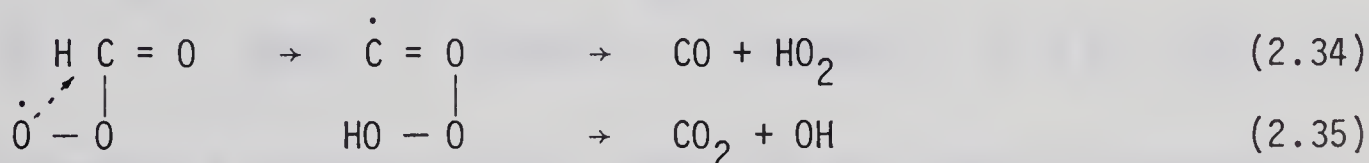
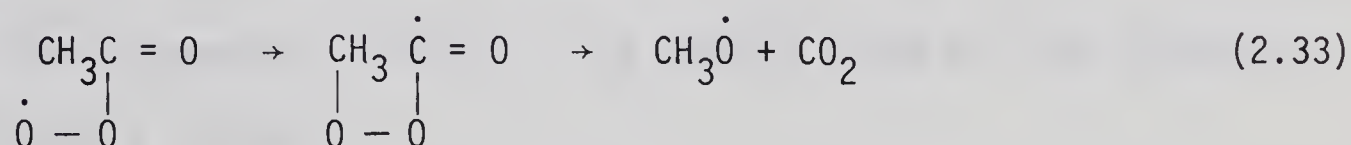
The acyl radicals formed by the oxidation of aldehydes in the branching reaction can react in a number of ways. They can decompose as follows:



These radicals can also react with oxygen.



However, these reactions have low steric factors compared to the decomposition reactions and mostly the $\text{H}\dot{\text{C}}\text{O}$ radical and to some extent the $\text{CH}_3\dot{\text{C}}\text{O}$ radical are likely to enter into reaction with oxygen. The acetyl and formyl peroxy radicals can decompose with initial isomerization.



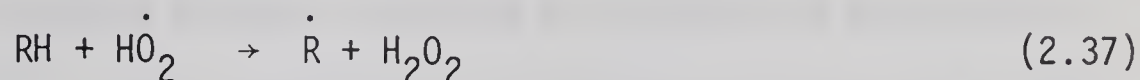
An alternative for these peroxy radicals would be to react with a hydrocarbon molecule forming acyl hydroperoxide. However, at higher temperatures, decomposition will prevail.

The hydroxy radical formed in the system reacts with a paraffin molecule.

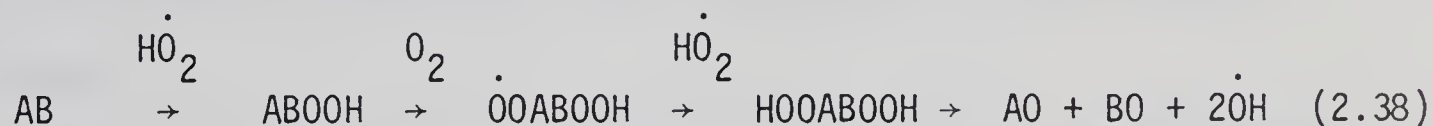


The fate and role of the hydroperoxy radical ($\text{H}\dot{\text{O}}_2$) is still a

matter of controversy. Some investigators suggested that it can attack a paraffin molecule especially in a fuel rich system as follows:



Others, including Knox do not believe the above is an important reaction. Knox^(9,10) quite recently made a bold attempt to explain the hydrocarbon oxidation reaction by considering the activities of the different free radicals. He suggested that the $\dot{\text{H}}\text{O}_2$ radical is quite inert, but is sufficiently reactive to combine with the olefins. A chain reaction is then started leading to the formation of oxygenated products and the transformation of the $\dot{\text{H}}\text{O}_2$ radical to $\dot{\text{O}}\text{H}$ radical. This transformation is basic to the theory of Knox, since his experimental results suggest that 80 per cent of the initial products of alkane oxidation are conjugate olefins by reactions of the type (2.3) and (2.4) which invariably produces the hydroperoxy radicals. The overall route for the transformation of the $\dot{\text{H}}\text{O}_2$ radical is



where AB denotes a conjugate olefin. Knox has very simply accounted for the negative temperature coefficient by suggesting that at that temperature region, the above mechanism fails and HO_2 becomes the major propagating species. At still higher temperatures, the reaction picks up again because of the thermal pyrolysis of hydrogen peroxide to $\dot{\text{O}}\text{H}$ radicals, which once again take up the propagating role.

Recently, Hughes and Simmons⁽¹¹⁾ studied the reaction of n-pentane with oxygen in the range 257 to 280°C at initial pressures which cover both the slow oxidation and cool flame regions. They obtained

60% of the initial products as acetone and found that cool flame formation is accompanied by relatively large amounts of olefins. Holtzmeier and Albright⁽¹²⁾ studied propane oxidation by introducing propylene in a reacting stream. As the concentration of propylene increased to 10%, the induction period decreased by 20% and the overall kinetics of the reaction increased. The induction period decreased at higher concentrations of propylene. No significant role of propylene, on the whole, was observed. Similar conclusions were drawn earlier by Satterfield and Wilson⁽⁴⁾. Lucquin and coworkers⁽¹³⁾ suggested that at temperatures 270° to 350°C, olefins are formed by a heterogeneous isomerization process which becomes mainly homogeneous in the negative coefficient zone.

2.3 EFFECT OF REACTION VARIABLES

The operating conditions for the partial oxidation reactions vary to some extent with the paraffin being used, the higher paraffins being more oxidizable than the lower ones. The range of operating conditions normally encountered in the laboratory or pilot plant are as follows:

Temperature	300 to 500°C
Pressure	0.2 to 15 atm
Paraffin to Oxygen Ratio	1:1 to 15:1
Residence Time in Reactor	0.1 to 10.0 sec

and up to several hours.

In general, lower pressures require higher temperatures and/or residence times. Higher pressures favour the formation of oxygenated compounds, and higher temperature promotes olefin formation, while higher oxygen to hydrocarbon ratio oxidizes greater amounts of initial hydrocarbons and

promote greater formation of carbon oxides and water. Runs at pressures below atmospheric and higher residence times are likely limited to the laboratory.

Duthie⁽¹⁴⁾, Dalla Lana⁽¹⁵⁾, Musgrove⁽¹⁶⁾ and Anderson⁽¹⁾ carried out experiments to determine the effects of temperature, pressure, residence time, and inlet gas composition on the vapour phase oxidation of n-butane at the University of Alberta between the years 1950 and 1966. Anderson designed and built a tubular reactor 0.625 inch diameter and 9 foot length of 316L stainless steel, with five sample points along the length of the reactor. Gas and wall temperatures were measured at different points along the reactor by thermocouples. The control of all reaction variables, temperatures, pressure and reactant flow rates, was accomplished by the use of either pneumatic or electronic controllers. Experiments were conducted at three temperature levels of 685°F, 705°F and 725°F, and indicated the dependence of the induction period on the inlet temperature. Runs were also made at four different inlet oxygen concentrations to study its effect on the overall reaction. The reactions gave a 60% conversion of the n-butane reacted to olefins for most of the runs. Only 10% of the n-butane that reacted went to carbon oxides. Of the remaining 30%, 10% went to lower molecular weight paraffins and 20% to oxygenated products. The oxygenated products consisted of aldehydes, ketones and alcohols. The gas temperature for any run remained fairly constant during the induction period and then increased rapidly to a peak temperature approximately 400°F above the inlet temperature. After the period of rapid reaction, the gas temperature decreased gradually because of heat transfer from the gas to the reactor wall. The period of rapid reaction during which the temperature shot up by about 400°F was

0.1 to 0.2 sec.

Quon, Dalla Lana and Govier⁽¹⁷⁾ obtained an increased yield of oxygenated products by an increase in the reactor pressure. An optimum pressure of 125 psia was obtained for the reactor at a residence time of 1.2 to 1.8 sec. operating at a temperature of 725°F and inlet n-butane to oxygen ratio of 1:1 in the presence of 90% nitrogen.

The effects of surfaces on the partial oxidation reaction is known, but its role is not clearly understood. Surface effects of importance include surface to volume ratio of the reactor, the nature of the surface, and the treatment or coating of the surface. The reactor wall in many cases can play an important role in the initiation and termination steps in the free radical reaction⁽¹²⁾.

Knox⁽¹⁸⁾ has recently postulated that considerable part, if not the whole of the minor products are formed in heterogeneous processes, which by consequence play a very important role in the range from 230 to 350°C and subatmospheric pressure. He arrives at this by way of explaining why the ratio of major to minor products is little affected by composition, total pressure, temperature or surface, while the distribution of minor products is highly sensitive to these parameters. The minor products by the definition of Knox are the oxygenated products and the major products are the olefins.

Euker and Leinroth⁽¹⁹⁾ oxidized n-butane in a flow reactor at 352-425°C and at pressures of 0.25 - 6.5 atm. Unlike Knox, they did not observe the major role being played by the surface. At 425°C and lower pressures, surface effects appeared to be important for some of the cracking products.

Albright⁽²⁰⁾ observed that the surface effects tend to decrease

as the pressure increases or as the diameter of the tubular reactors increase. The ratio of surface of the reactor wall to the mass of the reaction mixture appears to be a very important factor relative to surface effects. For pressures of at least 6 atmospheres and for reactors with diameters of 5 to 6 inches or greater, surface effects may be inconsequential and gas phase reactions would be controlling. Surface effects in industrial reactors are probably of minimal importance.

2.4 METHODS OF CONTROLLING THE REACTION

The hydrocarbon oxidation is almost nonselective. The conversion of the hydrocarbon is generally low and the reaction leads to the formation of a large number of oxygenated compounds, lower paraffins, olefins, carbon oxides and water. A large amount of gas has to be recycled and the separation of the complex mixture of gases is difficult and expensive. Optimizing the yield of the reactor is vital to the economy of the entire process. Efforts in this area were directed to initiation at lower temperatures, use of homogeneous catalytic additives, removal of the intermediates as they are formed and at controlling the temperature of the reactor.

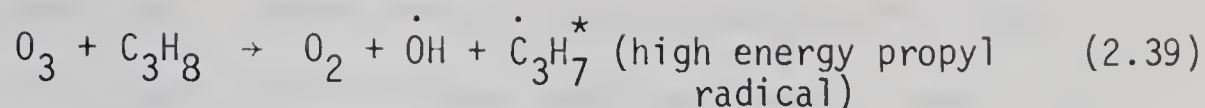
The hydrocarbon oxidation can be initiated at temperatures down to room temperature by supply of energy from outside, e.g., by photodissociation of certain chemicals which can supply free radicals, or by penetrating radiation such as r-rays which can generate free radicals in the system⁽⁸⁾. However, these lead to very small conversions and are useful in mechanism studies alone.

The effect of a large number of homogeneous catalytic additives such as NO_2 , Cl_2 , Br_2 , HCl , N_2 , etc. has been studied by several

investigators⁽²¹⁾. The overall effect of these additives has been to shorten or eliminate the induction period by facilitating the initiation of the active centres, or to decrease the temperature of ignition and reaction. This sometimes leads to an improvement in selectivity.

Rust et al⁽²²⁾ studied the effect of addition of hydrogen bromide on the oxidation of different hydrocarbons. It was observed that in the presence of a tertiary bond in the hydrocarbon molecule the main oxidation product is an organic peroxide; if there are secondary bonds, the main oxidation product is ketone, and a hydrocarbon with a primary C-H bond leads mainly to organic acids. Thus, the addition of HBr leads to a significant change in selectivity and the oxidation presumably follows a different course. The oxidation temperature decreased by 100-120°C. For example, the oxidation of *i*-C₄H₁₀ occurs in absence of HBr at 265°C while with 20% HBr it occurs at 155-165°C. Further investigations are needed to confirm these findings.

Schubert and Pease⁽²³⁾ studied the oxidation of methane, propane, butane and iso-butane in mixtures with oxygen in the presence of about 3 per cent ozone under static and flow conditions at temperatures of 25-50°C and 170-270°C. In the case of propane and butane, it was noticed that the addition of ozone eliminated the induction period completely. A mechanism with initiating reactions of a hydrocarbon molecule with ozone forming an alkoxy radical and a HO₂ radical was suggested. Kleimenov et al⁽²⁴⁾ in a study of ozone oxidation of methane indicated that the reaction proceeds by ozone decomposition to give oxygen atoms which subsequently react with the hydrocarbon molecule. Dardrin and Albright⁽²⁵⁾ suggested the formation of a high energy propyl radical and an $\dot{\text{O}}\text{H}$ radical by reaction of propane with ozone.



Slavinskya et al⁽²⁶⁾ obtained higher conversion of n-butane and better selectivity for aldehydes in presence of ozone in the reaction mixture. In all cases, the induction period and the ignition temperature generally decreased.

Mitchel and Locke⁽²⁷⁾ allow a small amount of paraffin and air to react. This mixture which contains free radicals at a high concentration is injected as a side stream into the reactor. The side stream initiates reaction in the mainstream and an increase in selectivity has been observed. Jones and Fenske^(28,29) obtained high yields of oxygenated products in a tubular reactor by controlling the reactor temperature by the introduction of inert solid particles as heat sink in the system.

Albright⁽³⁰⁾ quoted an industrial patent for an isothermal reactor. In one example, the hydrocarbon stream was preheated to 475°C and the oxygen stream was not heated. The temperature in the reactor was 500°C. In another example, both hydrocarbon and oxygen feeds were heated to 320°C and the reactor operated at 525°C. The presence of inert gases such as NO₂, CO and CO₂ was claimed to be beneficial in controlling the rate of the reaction.

Oberdorfer and Winch⁽³¹⁾ studied the oxidation of methane in a motored engine at a compression ratio of 40:1. The motored engine offers a means of effective control of the reaction because of its cyclic operation where high temperatures and pressures occur for very short periods of time and the reaction can be initiated and quenched easily by the proper selection of the operating variables. Methanol, formaldehyde and formic acid were the chief chemical products formed under nearly all

conditions of operation. Carbon monoxide and hydrogen were formed concurrently in an amount under optimum conditions nearly equal to the total C_1 chemical products. Of the approximately 6% methane converted, approximately 40% formed C_1 oxygenated products, 33% formed CO and essentially no CO_2 was formed. Of the oxygen originally charged, approximately 44% was consumed in the reaction. Methane was obtained from a natural gas stock and 8% concentration of oxygen in 75% methane was found to be the optimum. The addition of 0.5% NO_2 in the gas nearly doubled the production of the chemicals, but shifted the optimum concentration of oxygen to 5-6%.

Gudkov⁽³²⁾ used a cold hot tube reactor for the oxidation of methane and propane. This is an annular reactor where the surface of the outer tube is hot (600 to 700°C) and that of the inner tube is cold. Gas passes through the annulus and water is circulated through the inner tube with a water film flowing past the outer surface of this tube. As a result of the great temperature gradient and convective flow, intensified diffusion exchange takes place in the annular space between the layers of gas at the hot and cold walls. Formaldehyde and other intermediates get dissolved in the water film and removed from the reactor with the water stream. Accordingly, in contrast to the method used in the partial oxidation in an ordinary tube in which the molecules of the intermediates formed must remain in a zone with reaction temperature for the entire length of time that is required for complete reaction, in the cold hot tube reactor they are removed from the reaction zone as they are formed. This should lead to an increase in the yield of oxygenated compounds and a decrease in the relative amount of by-products of the reaction. Gudkov obtained an increase of formaldehyde concentration

5 to 6 times for methane and 2 to 3 times for propane in a cold hot tube as against in an ordinary tubular reactor under comparable conditions.

2.5 TRANSPORTED BED REACTORS

Transported bed reactors have been used in industries for a long time, but little published information is available on their operations. In a transported bed reactor (henceforth referred to as TBR), a catalyst, an inert or a reacting solid is carried as a powder by gas through a long, narrow pipe line at velocities of 20 to 100 ft/sec. Generally, the solid is dilute in phase (less than 1% by volume) and can range in size from 40 to 1000 microns in diameters. Under these conditions, there is little backmixing of either gas or solids and the terminal velocity of solids through the gas is low compared with the absolute velocity of the gas; therefore, the contact time of the reactor can be accurately fixed. Also, the gas is fully turbulent and the solids can be considered to be uniformly dispersed through the cross-section of the pipe. Lower gas velocities complicate the residence time distribution and the uniform dispersion of the solids, but provide greater contact time between the solids and the gases for reaction and heat transfer. As the reaction proceeds with evolution of heat, the solid particles take up the heat of reaction and can maintain an essentially isothermal condition. With proper selection of the variables, it is possible to have the reactor temperature follow a certain chosen optimum path.

An exploratory study of TBR was made by Jepson and coworkers⁽³³⁾ for the thermal cracking of sodium bicarbonate. Dalla Lana⁽³⁴⁾ and Themelis and Gauvin⁽³⁵⁾ used this type of reactor for the direct reduction of iron oxide powder with hydrogen. Paetkau⁽³⁶⁾ used a TBR for

the partial oxidation of o-xylene. The solid particles were fed to a horizontal section of pipe by a rotary solids feeder and then conveyed upwards by the reacting gases. Solid particles of average diameter 50 μ , density 131 lb/ft³ were used at solids to gas loading ratios of 8 to 23 at a reaction temperature of 750°F. Othmer⁽³⁷⁾ has described a number of applications for TBR in industries.

Jones et al^(28,38) used a reactor which they describe as a "raining" solids reactor where noncatalytic solid particles rain down against a countercurrent stream of gases. The solid particles are conveyed to the top of the reactor by dry steam. The reactor section is a 26 inch length of 1.5 in. diameter schedule 80 steel pipe and the operating conditions are 570°F to 1200°F at pressures ranging from atmospheric to 60 psig. A large number of solid particles such as fused alumina (125 μ), sand, glass beads (300 μ), mullite (300 μ), and zircon silicate (300 μ) were used at solids to gas loading ratios of 5 to 10. The oxygen was introduced at multiple points which also helped check the rise in temperature. The unit is operated in such a way that the oxygen added at one point is all consumed before the next oxygen inlet is reached. A large number of hydrocarbon stocks were investigated. At a reaction temperature of 400° to 420°C and a pressure of 50 psig, n-butane gave oxygenated compounds as the major products. At atmospheric pressure and the same temperature, olefins predominate.

The initiation of the reaction was found to be a function of the total pressure of the system, the solids surface area present, the quantity of diluent nitrogen and the geometry of the reactor. For the oxidation of ethane at 50 psig, the oxidation temperature was 100°C higher when 80-100 mesh particles were used compared to 35 to 40 mesh

particles. This difference was apparently due to the larger surface area present for the smaller particles. This effect was not observed for the higher, more reactive hydrocarbons.

2.6 PRODUCT ANALYSIS

The most powerful single tool for the analysis of the combustion products is vapour phase gas chromatography. Since 1960, research workers in the field of hydrocarbon oxidation have almost exclusively used the gas chromatograph to analyze the products of the reaction⁽³⁹⁾. A number of instruments such as mass spectrometer, infrared spectrometer and N.M.R. have also been used in conjunction with the gas chromatograph. The coupling of a mass spectrometer with the gas chromatograph is very useful, as it provides simultaneous measurement and identification of the host of products that are formed in the hydrocarbon oxidation⁽⁴⁰⁾. Norrish and Porter⁽⁴¹⁾ have used a gas chromatograph which takes samples directly from the reactor and the products are analyzed simultaneously in multiple columns using the same detector. Varkey and Sandler⁽⁴²⁾ have studied the oxidation of 2-methyl butane during the induction period using a flame detector in the gas chromatograph. The flame detector is about a thousand times more sensitive than the thermal conductivity detector usually employed, and is eminently suitable for studying the reaction during the initiation period.

2.7 SPECIAL EXPERIMENTAL TECHNIQUES

The usual method of studying the reaction is to determine quantitatively the product distribution as the reaction proceeds. The earlier studies almost exclusively measured the pressure change with

the reaction. The change of temperature has also been used to study the reaction. Another interesting and very useful method seems to be the use of isotopes, employed by Russian workers and in increasing use now in hydrocarbon oxidation studies⁽⁴³⁾. Since the labelled atoms may be traced in the product, some of the finer details of the reaction can likely be elucidated.

2.8 SUMMARY

A vast amount of work has been reported in literature on the mechanism of the reaction of hydrocarbons with oxygen and the effects of different variables such as temperature, pressure and surface on the course of the reaction. Two major contenders emerge from the mechanism study in the last decade: the aldehydic mechanism of Semenov and Shtern and the olefinic mechanism of Knox. The suggestion of Knox that all the oxygenated products in the reaction are derived from heterogeneous reactions on the surface also merits serious consideration and has received considerable attention in recent literature.

The amount of work on the improvement of selectivity of the reaction products is rather limited. The pioneering works of Oberdorfer and Winch in a motored engine reactor, of Gudkov in a cold hot tube reactor and of Jones and coworkers in a raining solids reactor are very worthwhile efforts in this direction. Further engineering research is warranted to obtain successful tools in controlling the hydrocarbon oxidation reaction and to improve the selectivity to useful products.

CHAPTER III

SCOPE OF THIS WORK

The present work is a continuation of the overall study of the gas phase oxidation of hydrocarbons. A tubular reactor used earlier in this laboratory was modified to operate both as a homogeneous reactor and as a transported bed reactor. Solids feed and separation systems were designed and built. The solids were introduced into the system by a rotary solids feeder and were separated at the exit by a cyclone followed by a filter.

A mathematical model was formulated to represent the transported bed reactor system with temperature distribution in the solid particles. Numerical method for solving the system was developed and the solution obtained in order to evaluate the effects of particle material properties, the particle diameters and the gas to solid loading ratios on the heat removal efficiency of the system.

Runs were made in the homogeneous reactor to study the effect of inlet temperature and inlet n-butane to oxygen ratios on the overall oxidation process and on the product selectivity. The product selectivity data were used to suggest possible mechanisms for the reaction.

A number of runs were made to study the effect of adding solids in a transported bed reactor. The selectivity and overall oxidation of n-butane and oxygen, and the effect on the temperature profile in the reactor were compared with those for the homogeneous runs.

Parameters were estimated for the two kinetic models using the overall conversion and temperature profile data for homogeneous runs. The same models were used to predict the overall conversions and temperature profiles for the transported bed reactor.

CHAPTER IV

EXPERIMENTAL DETAILS

4.1 EQUIPMENT

A schematic diagram of the equipment and the associated instrumentation to control the feed rates, the reactor pressure and temperature, and the preheater temperatures is shown in Figure 4.1. The air and n-butane flow systems, the air and n-butane preheaters, and the temperature and flow control systems have been described in detail in an earlier investigation (1), and will not be discussed in great length here.

The reactor is a 9 foot length of 316L stainless steel tubing with inside and outside diameters of 0.625 inch and 1.25 inches, respectively. The gas preheaters are made of 3/8 inch 316 stainless steel. Both the reactor and the preheaters are heated by cylindrical Kanthal heaters and insulated by Johns Manville asbestos insulation. The n-butane is fed to the preheater as a liquid by nitrogen pressure. Air is taken directly from a compressed air line, after being passed through a pressure regulator and strainer to remove moisture or oil.

The solids preheater is a cylindrical tank 8 feet in length and 7.5 inches in diameter, fabricated from 1/8 inch mild steel sheet. The bottom section is made conical with an inside diameter of 2 inches to join with the solids feeder. The tank is surrounded by a tubular furnace made from Nikrothal 80 wire B and S gauge #11 (0.091 inch diameter) supported on Kanthal Y4-1286B bricks and insulated by fire-bricks.

The solids feeder, flange connected to the bottom of the solids heating tank, is a rotary valve. Each revolution of the rotor

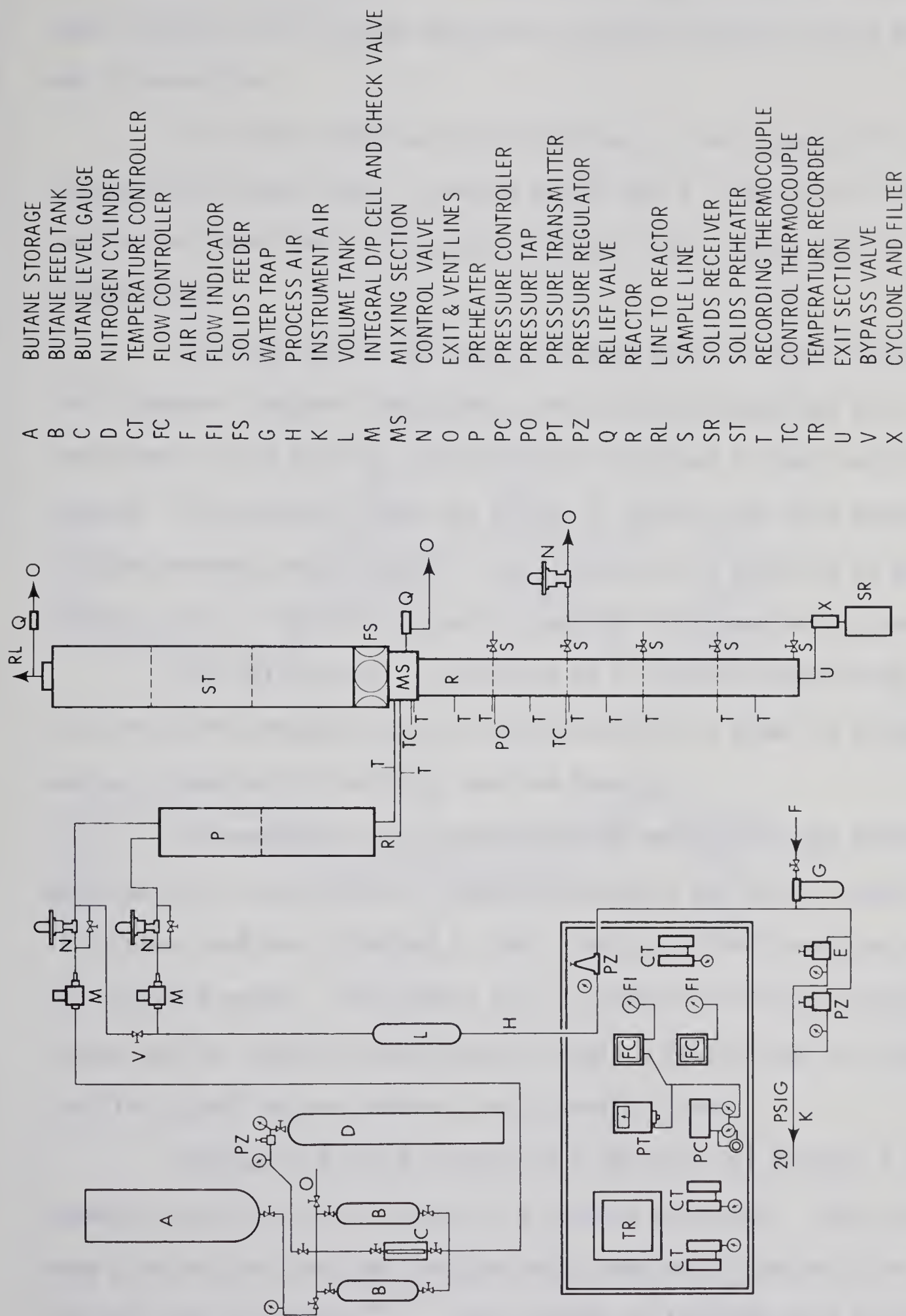


FIGURE 4.1 SCHEMATIC LAYOUT OF EQUIPMENT

transfers a fixed volume of solids from the tank to the solids discharge cone. The clearance between the rotor and the valve is very small (0.005 inch) in order that the valve may hold the solids when not in operation.

The valve rotor was machined from a 6 inch length of 4 inches diameter mild steel block. Grooves 0.045 inch x 0.045 inch in cross section were machined in the outer surface of the rotor, with a total of 136 slots.

The housing for the rotor was made from a 6 inch section of 4 inch diameter standard steel pipe. The solids entrance and exit ports are welded to the housing. An end plate is bolted to each end of the housing. The purpose of the end plates is to seal the unit and to provide bearings for the shaft. An o-ring seal is required to make the unit gas tight. The o-ring seal is made of high temperature graphite.

The valve shaft is connected to a variable speed drive. Heating wires were wrapped around the valve housing in order to prevent unequal expansion of the rotor and the housing.

Thermocouples are incorporated to measure the gas and wall temperatures in the reactor. Samples are taken out of the reactor at five points and are collected in small stainless steel bombs by actuating solenoid valves. The sample line is made of 1/8 inch stainless steel tubing and the sample stream passes through a filter made of sintered stainless steel before entering the solenoid valves.

The gas and solid streams in a TBR come out through a 1/2 inch diameter stainless steel tubing to a cyclone separator. The cyclone is made of mild steel and was designed with some modification of the specification given by Perry⁽⁴⁴⁾. The cyclone is followed by a filter made

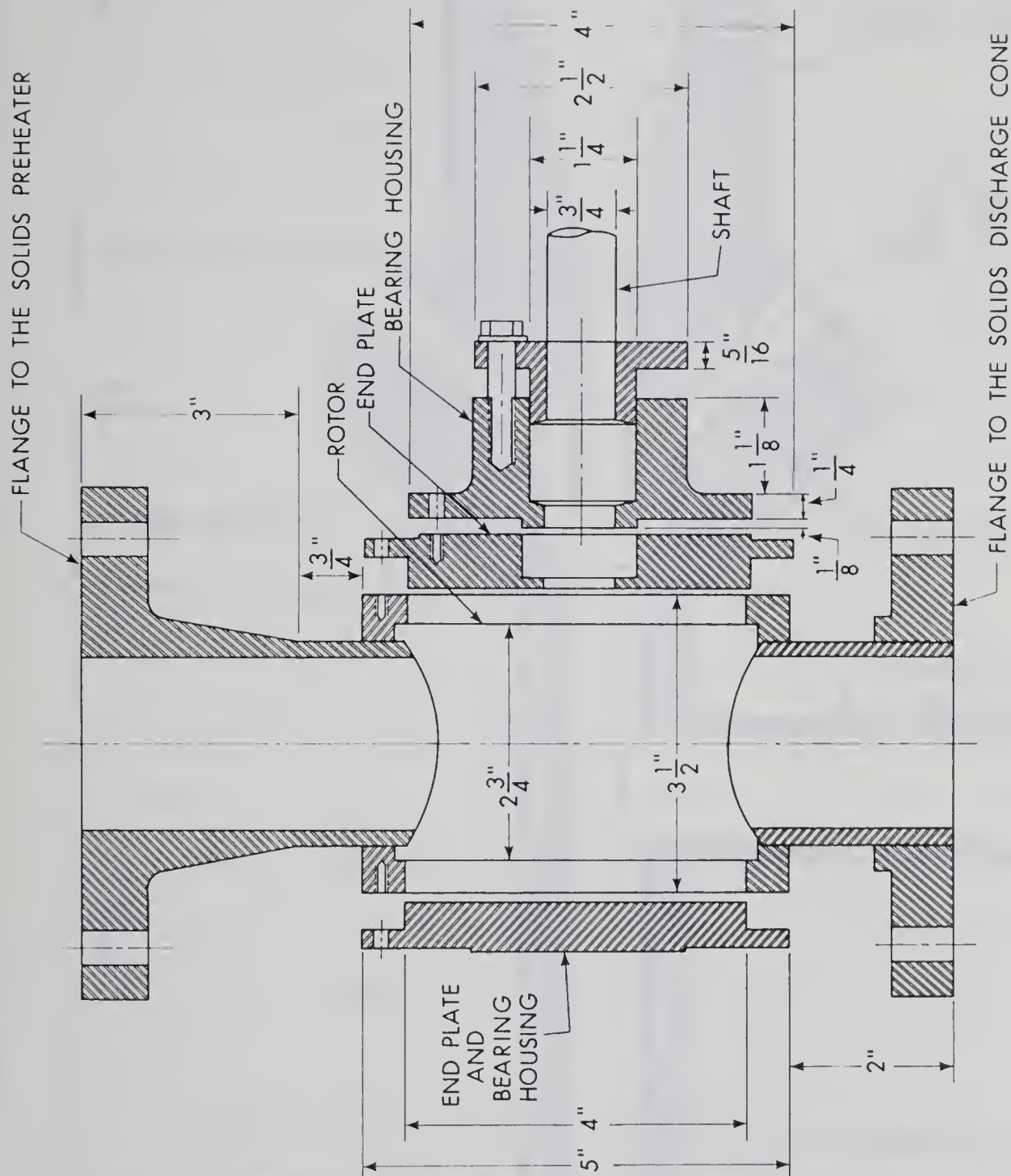


FIGURE 4.2 SOLIDS FEEDER

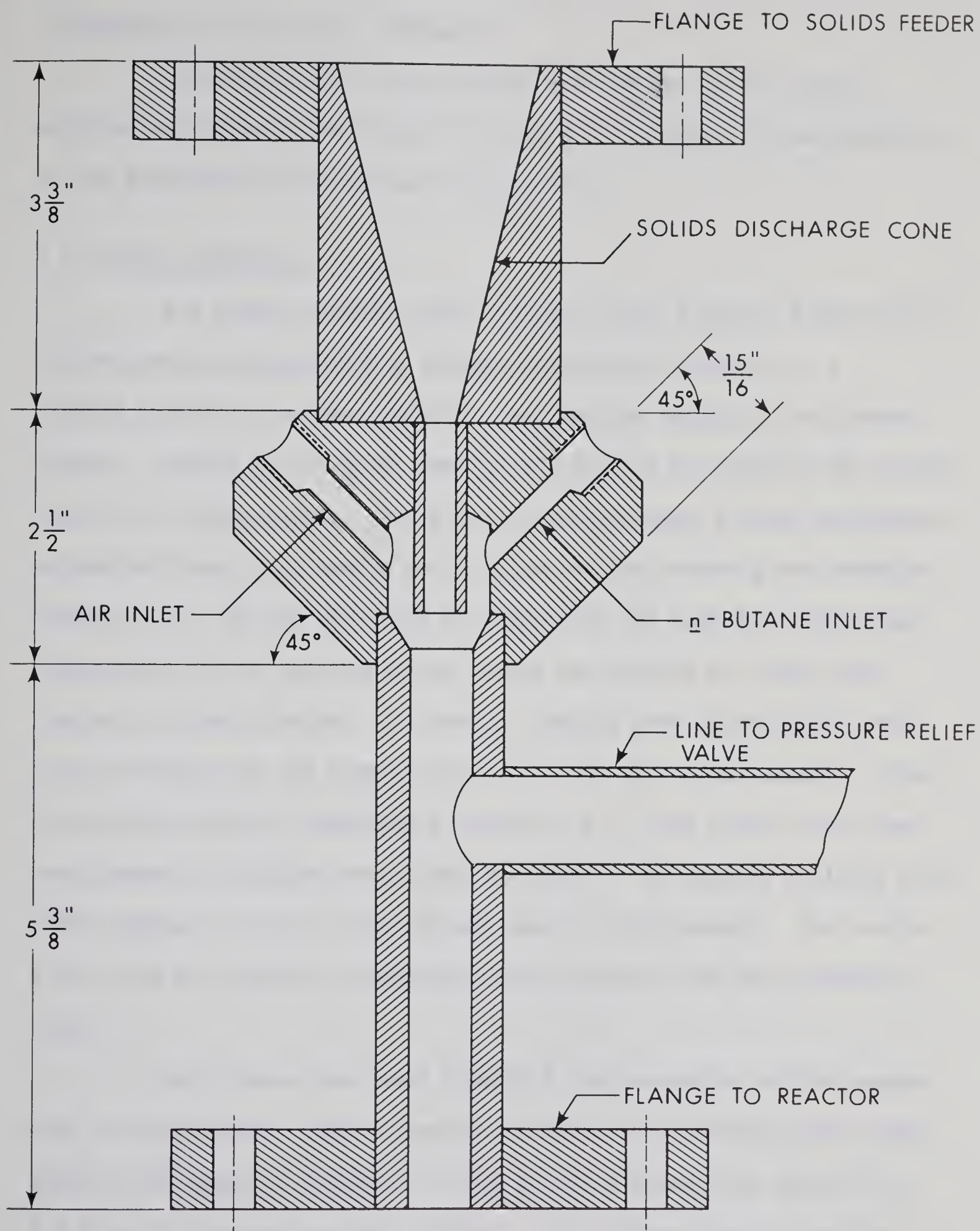


FIGURE 4.3 MIXING SECTION FOR GAS AND SOLIDS

of stainless steel screen, 400 mesh.

Diagrams of the solids feeder and the gas-solids mixing section are presented in Figures 4.2 and 4.3. Details of some features of the equipment are presented in Appendix A.

4.2 PRODUCT ANALYSIS

All product samples were analyzed using a Burrel Model KD gas chromatograph equipped with a thermal conductivity detector. A Sargent millivolt recorder model SR recorded the output of the chromatograph. Helium at air inlet pressure of 40 psig was used as the carrier gas for all the analyses. The helium passed through a drier cartridge of molecular sieve 5A to remove any moisture before entering the chromatographic unit. Helium flow rate was regulated for both the carrier and reference sides by Nupro metering valves and checked by timing soap bubbles in a gas burette. All product samples were injected into the column through the gas sampler built into the gas chromatograph. Since the sample contained condensable products, all lines before the column were heated by wrapping around heating tapes. The samples analyzed were under pressure and the injection was done by displacement. The sample size could be changed by changing sampler tubes of 1/8 inch stainless steel.

Two columns were used to effect the separation of the components in the mixture. Both columns were made from 3/16 inch soft copper tubing with Swagelok fittings on both ends and wound into spirals to fit into the temperature bath cabinet. The columns, their operating conditions, and the components separated are as follows:

Column 1: A 12 ft column packed with 80 to 100 mesh Porapak S made by Waters Associates.

Components separated: Paraffins, olefins, oxygenated hydrocarbons, carbon oxides and water.

Column Temperature: 50°C for the first 6 minutes followed by 10°C/min rise to 150°C, 10°C/min rise to 200°C after 30 minutes from the beginning.

Carrier Flow Rate: 42 cc/min

Reference Flow Rate: 40 cc/min

Detector Current: 200 ma

Gas Sampler: 12 inch long 1/8 inch tube, 0.75 cc volume

Column 2: A twelve ft column packed with high activity charcoal 40 to 60 mesh for the first six ft followed by an equal length of molecular sieve type 13X.

Components separated: Hydrogen, oxygen, nitrogen, methane and carbon monoxide.

Column Temperature: 40°C

Carrier Flow Rate: 35 cc/min

Reference Flow Rate: 30 cc/min

Detector Current: 250 ma

Gas Sampler: 5.5 inch long, 0.28 cc volume

The components were identified by their retention times. The retention time of a component is the time taken from sample injection to the maximum point in the peak. Retention times for the various components and examples of the chromatograms for each chromatographic column are reported in Appendix B.

4.3 OPERATING PROCEDURE

The preheater and reactor systems for a homogeneous run were first heated for a few hours with air only in the system. Before the

introduction of n-butane in the system, the pressure of the reactor was raised to about 30 psig. This eliminated sudden build up of pressure when n-butane was introduced in the system and also allowed a rapid attainment of a steady pressure of 40 psig used in the study.

Before a TBR run was made, it was necessary to heat the solids for a long period of time. The solids were first heated for seventy-two hours and then the air streams turned on as in a homogeneous run. The heating was allowed to go on for another twenty-four hours in order to ensure steady solids temperature. A small leak of air at the top of the solids tank was found to aid in enhancing the solids heating rate.

Samples were taken in each run at steady state. Steady state was considered achieved when a steady temperature profile was obtained, as recorded by the multipoint temperature recorder. The samples were stored in an oven at 110°C to be analyzed in a gas chromatograph.

4.4 CALIBRATION OF EQUIPMENT

Calibration of the integral D/P cells for n-butane and air flow rates, and the pressure transmitter was carried out prior to the start of the experimental program. Calibration procedures and curves are presented in Appendix C. The calibrations were checked at random intervals during the progress of the experimental investigation.

4.5 EXPERIMENTAL DIFFICULTIES

A number of serious experimental problems were encountered during the progress of this investigation. This section describes some of them. The development work needed to solve those problems is also included.

The development of a satisfactory method of feeding the solids posed a major problem. The high temperature and pressure both act contrary to the satisfactory performance of any solids feeder.

Initially, an orifice feeder with solids heating in spiral tubes was investigated. The orifice feeding accomplished by applying differential pressure in the solids tank was found to be very uniform and highly reproducible, but the heating system was not satisfactory. The possibility of solids plugging always remains in a gas solids system, and no satisfactory solution could be possible once it occurs in spirally coiled tubes.

The method of heating was therefore changed to heating in batch in a tank. This, however, posed a problem for orifice feeding because of the difficulty in the design and operation of a valve which would operate satisfactorily.

The use of a screw feeder was explored, but was abandoned because of the nonuniformity of flow.

The rotary solids feeder finally adopted for the system has been on the whole very satisfactory. The solids flow is uniform and reproducible. Initially, there was jamming of the rotor. This was likely due to unequal expansion of the rotor and the housing, and was remedied by heating the housing. The solids feeder operates with a lot of vibration and a strong foundation is necessary.

In the earlier evaluation of the solids feeder, the solids backflowed and came out through the entrance lines. This happened once because of a leak in the upstream section of the air line and again because of a pressure build up in the reactor. Care has to be taken to avoid such incidents.

The solids separation system also gave some serious trouble. The initial cyclone was not adequate and there was appreciable carry over even from a filter used at that time. A small amount of solid particles passing for a short time can significantly erode the exit valve in the reactor. The clearance between the solids rotor and housing is small, but even then some solids can pass through when there is a sudden change in pressure and flow rates in the system. Some care has to be taken to avoid sudden change in these quantities when solids are in the system. The disturbance during the start-up was eliminated by raising the pressure of the reactor to 30 psig before the introduction of n-butane. The shut down also needs some manipulation and adjustments.

CHAPTER V

EXPERIMENTAL PROGRAM

5.1 REACTION VARIABLES

Preliminary evaluation of the homogeneous reactor suggested gas temperature profile as an index to the overall reaction and the product selectivity. The inlet temperature affected the length of the induction period without significantly affecting the further course of the reaction. Increase in oxygen concentration led to a higher overall conversion of n-butane, but a lower yield of the oxygenated compounds. Attempts were directed at improving the selectivity and also to obtain samples at different regions of oxidation so as to be able to evaluate the progress of the reaction.

Homogeneous runs were conducted at three temperature levels of 687°F, 702°F and 708°F, and at four different hydrocarbon to oxygen ratios of 14, 11, 8.7 and 7.7. In all the runs, oxygen was obtained from air which resulted in a definite percentage of nitrogen in the reaction stream.

Details of the experimental runs are given in Table 5.1. The experimental temperature profiles are presented in Table D.1 in the Appendix.

The runs in the transported bed reactor are described in Section 7.3.1.

5.2 RAW MATERIALS

The experimental runs were made with C.P. grade n-butane supplied by Matheson of Canada Ltd. Chromatographic analysis of several samples gave a purity of over 99.5 per cent. The rest were propylene

TABLE 5.1

Experimental Run Details

RUN NO.	INLET TEMP. °F	PRESSURE psia	n-BUTANE: OXYGEN	RESIDENCE TIME sec	INLET REYNOLDS NUMBER
60	685	53.6	14.0	1.41	6358
61	695	53.7	11.0	1.37	6088
62	695	53.7	8.7	1.25	6199
63	702	53.6	6.9	1.16	6154
64	692	53.6	7.75	1.42	5402
65	687	53.5	7.37	1.23	6072
66	708	53.4	7.79	1.21	6080
67	684	53.6	5.73	1.56	4446
68	684	53.7	8.01	1.43	5357

and i-butane.

The oxygen for the reaction came from air. Analysis of the air revealed no trace compound.

The solid particles used in the transported bed reactor were silicon carbon powders supplied by Norton Company of Canada. The physical properties of these powders are given in Appendix A.

5.3 CHROMATOGRAPHIC ANALYSIS

All product samples were analyzed in a Burrel Gas Chromatograph. The components of the samples were identified by their retention times. The retention times for each component were determined for each component individually and then checked by running several known mixtures of the components. The retention times for each component are given in Table B.1.

The peak area for each component was determined by multiplying the peak height by the width at half the height. This was converted to molar composition by using a relative response factor as described by Rosie and Grob⁽⁴⁵⁾ and Messener et al⁽⁴⁶⁾. As the response factors are valid at constant temperature, and temperature programming was used in the present work, correction factors were obtained and these are presented along with the retention times in Table B.1.

CHAPTER VI

HOMOGENEOUS REACTOR: RESULTS AND DISCUSSIONS

6.1 Introduction

The performance of the equipment and the associated gas chromatograph has been reviewed. The experimental temperature profiles and the overall conversions have been plotted and the effects of inlet temperatures and inlet n-butane to oxygen ratio discussed. The dependence of the formation of different products on the same variables is enunciated with the help of plots of selectivity versus residence times. The conclusions formed thereby are further augmented by considering the reaction at low residence times and low conversions. A qualitative description of a possible mechanism that may be taking place is presented.

Two simplified kinetic schemes are proposed to describe the temperature profiles and the overall conversions of n-butane and oxygen in the reactor. The parameters of the models are estimated by using a numerical method. The models are tested by using them to predict the temperature profiles and conversions for a number of runs in an earlier work in this laboratory.

6.2 Equipment

The performance of the equipment as a whole was satisfactory. There was a maximum error of ± 1 per cent of the weight rate of flow of n-butane and air, because of a $\pm .5$ per cent deviation on the recorder chart. Sensitivity analyses show that this, however, can introduce an error of $\pm 10^\circ\text{F}$ in the maximum temperature attained. The reactor pressure was maintained fairly constant and no significant effect was observed for the ± 1 per cent deviation that occurred in the different

runs. The preheater temperature controller varied by $\pm 2^{\circ}\text{F}$. This introduces a fluctuation in the maximum temperature by $\pm 40^{\circ}\text{F}$. The reactor temperature controller was used mainly in preheating the reactor and was not normally effective otherwise. The observed $\pm 50^{\circ}\text{F}$ variation in the maximum temperature did not apparently introduce significant variations in the product distribution.

6.3 Product Analysis

Quantitative analysis of the reaction products was made by the use of relative response factors as described by Messener and coworkers (46). In order to check the accuracy of the method, a test sample was prepared and analyzed on the gas chromatograph. Results of the test sample are presented in table 6.1. Use of relative response factor limited the error within about ± 5 per cent of the true value as compared to ± 10 per cent if the area per cent is assumed equal to the weight per cent. The relative response factor for water given by Rosie and Grob⁽⁴⁵⁾ as 0.21 was found to be in considerable error. A new and corrected value of 0.31 was obtained and used in the quantitative analysis. The response factors for methanol and ethanol were also slightly

TABLE 6.1

Test Sample with Compositions Calculated Using
Relative Response Factors

Compound	True wt %	True Mole %	Observed Area %	Calculated Mole %
Water	8.81	24.54	8.1	23.64
Methanol	7.66	12.0	8.33	12.35
Ethanol	9.48	10.32	9.63	10.35
Propionaldehyde	15.04	12.98	13.89	13.28
n-Propanol	14.24	11.88	15.70	12.74
Methyl ethyl ketone	19.74	13.73	20.86	14.06
Diethyl ketone	25.0	14.55	23.40	13.53

out and were corrected. The response factors are generally obtained at constant temperatures. Since temperature programming is used in the present analysis, correction factors were calculated for each component, because the peak areas generally increase at elevated temperatures.

The analysis of the actual reaction mixture is very complicated because of the number of components and of the wide range in proportions in which they are present. The areas of the peak were calculated by the height-width method. There are four major areas of indeterminate errors in the measurement of peak areas by this method: placement of the base line, measurement of height from base line, positioning of the measuring instrument at a predetermined height, and measurement of the width. Harris and Kratochvil⁽⁴⁷⁾ combined all four errors statistically for peaks of constant area but of varying height to width ratios and obtained a minimum in the relative error at ± 2 per cent at a peak height to width ratio of 3. The relative error increases quite sharply at all other ratios, especially at lower ratios.

The major components in the reacting mixture are air and n-butane. The peak height to width ratio for air peak is about 40 and both the air and n-butane peaks are attenuated by a large amount. Besides, most of the oxygenated compounds are present in small amounts and have low peak height to width ratios. These factors introduce uncertainties in the analysis of the reaction products and would be responsible for the relatively poor oxygen balances of 80 to 100 per cent. The carbon and hydrogen balances are mostly bound within 95 to 100 per cent.

Analysis of a gas sample which contained a very large amount of one component relative to the others gave excellent reproducibility. A

standard natural gas sample supplied by Phillips Petroleum Company was obtained from another laboratory⁽⁴⁸⁾. Table 6.2 shows that the results obtained in the three laboratories are in good agreement.

TABLE 6.2
Analysis of a Standard Gas Sample

Component	Phillips	Energy Resources Conservation Board	Present Work
He, O ₂ , N ₂	6.02	6.05	6.06
Carbon dioxide	1.32	1.32	1.26
Methane	71.50	71.59	71.50
Ethane	7.33	7.10	7.40
Propylene	0.02	-	0.03
Propane	5.95	5.92	6.03
Isobutane	3.00	3.01	2.98
<u>n</u> -Butane	2.90	3.02	2.85
<u>iso</u> -Pentane	0.98	0.99	0.95
<u>n</u> -Pentane	0.98	1.00	0.97

6.4 Experimental Results

6.4.1 Temperature Profiles

Temperatures of the reacting gas stream were measured by nine thermocouples along the length of the reactor. All temperatures are listed in table D.1 in the appendix.

For any experimental run, the gas temperature first decreases and then increases very sharply, followed by a gradual decrease again. The initial decrease takes place for the length of the induction period

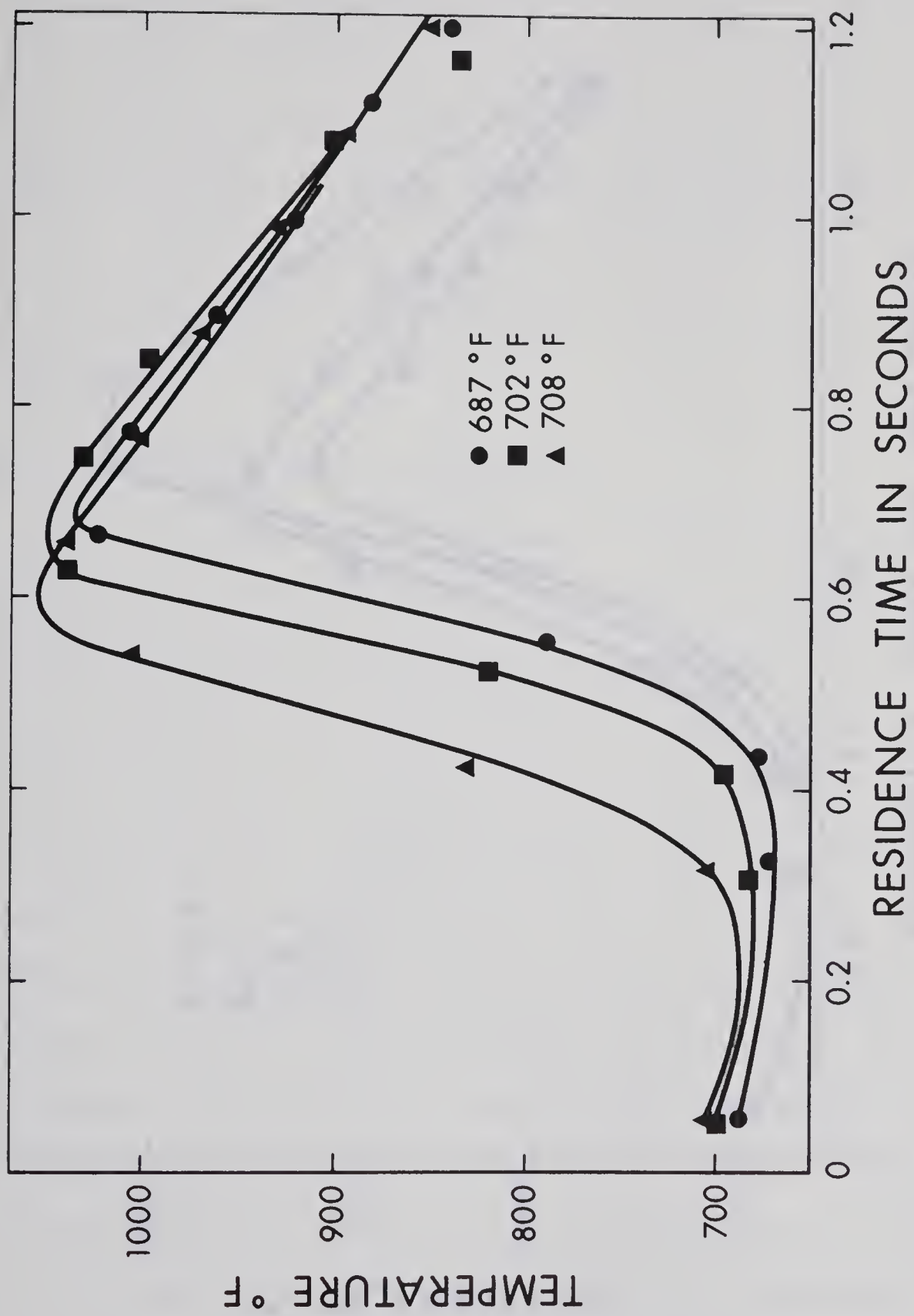


FIGURE 6.1 REACTOR TEMPERATURE PROFILES - EFFECT OF INLET TEMPERATURE

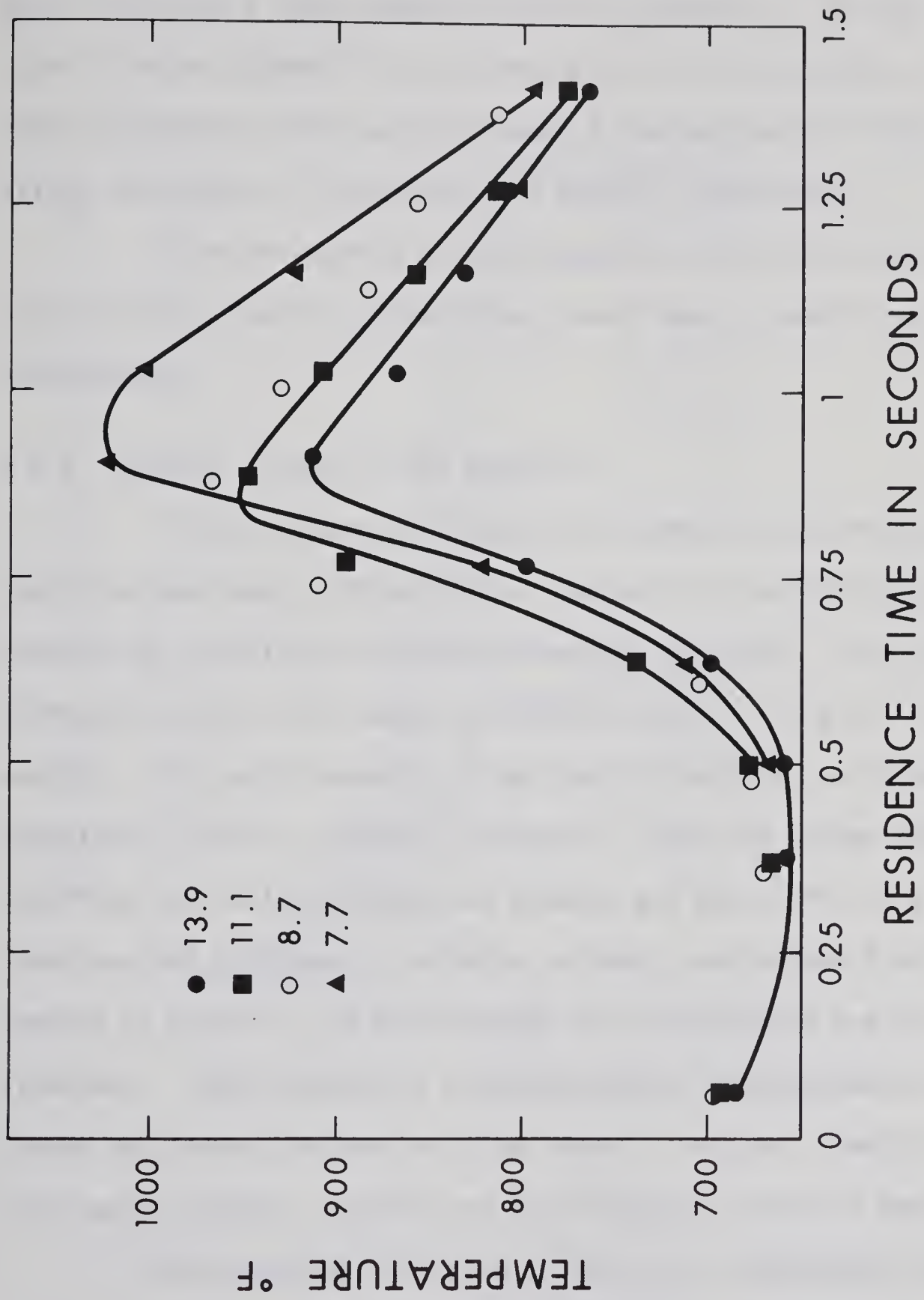


FIGURE 6.2 REACTOR TEMPERATURE PROFILE - EFFECT OF
INLET MOLAR RATIO

by heat loss to the surroundings. The increase in temperature at the end of the induction period is due to a very rapid rise in the reaction rate which liberates a large amount of heat of reaction. The gas temperature rises by about 300-400°F in a period of 0.1 to 0.15 seconds. Any thermocouple located at this section showed a fluctuation of $\pm 50^\circ\text{F}$ due to slight variations in flow rates and control temperatures.

After the period of rapid reaction, very little reaction takes place and the reacting stream slowly cools down by heat loss to the surroundings.

6.4.2 Products Formed in the Reaction

A large number of products are formed in the reaction. The study has been made with particular emphasis on the distribution of these products as affected by different reaction variables. For each run, five different samples were taken at different points along the length of the reactor. The major products of the partial oxidation of n-butane are paraffins, olefins, aldehydes, alcohols, water and carbon oxides. The paraffins are mostly methane and ethane, and the olefins are ethylene, propylene and n-butenes. The major alcohols are methanol and small amounts of ethanol, and formaldehyde and acetaldehyde are the principal aldehydes. Small amounts of propionaldehyde, acetone, methyl ethyl ketone and diethyl ketone are also formed. Propane, 2-methyl butane, n-pentane, propanol, butanol and butyraldehyde have also been isolated.

The method of reduction of the gas chromatographic data is outlined in Appendix E. The computer program and the results are also presented in Appendix E.

6.4.3 Effect of Reaction Variables

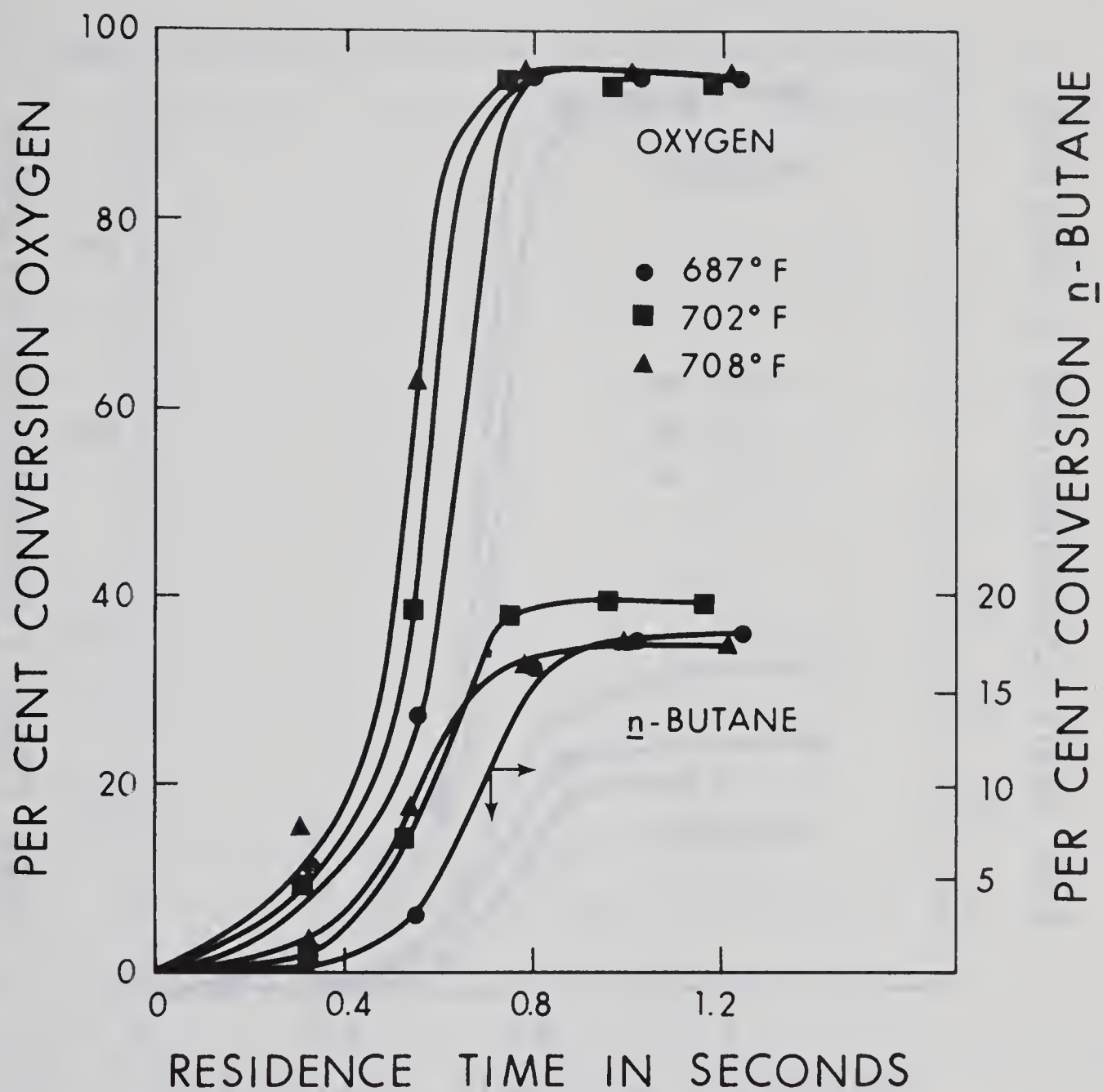


FIGURE 6.3 OVERALL CONVERSIONS - EFFECT OF INLET TEMPERATURE

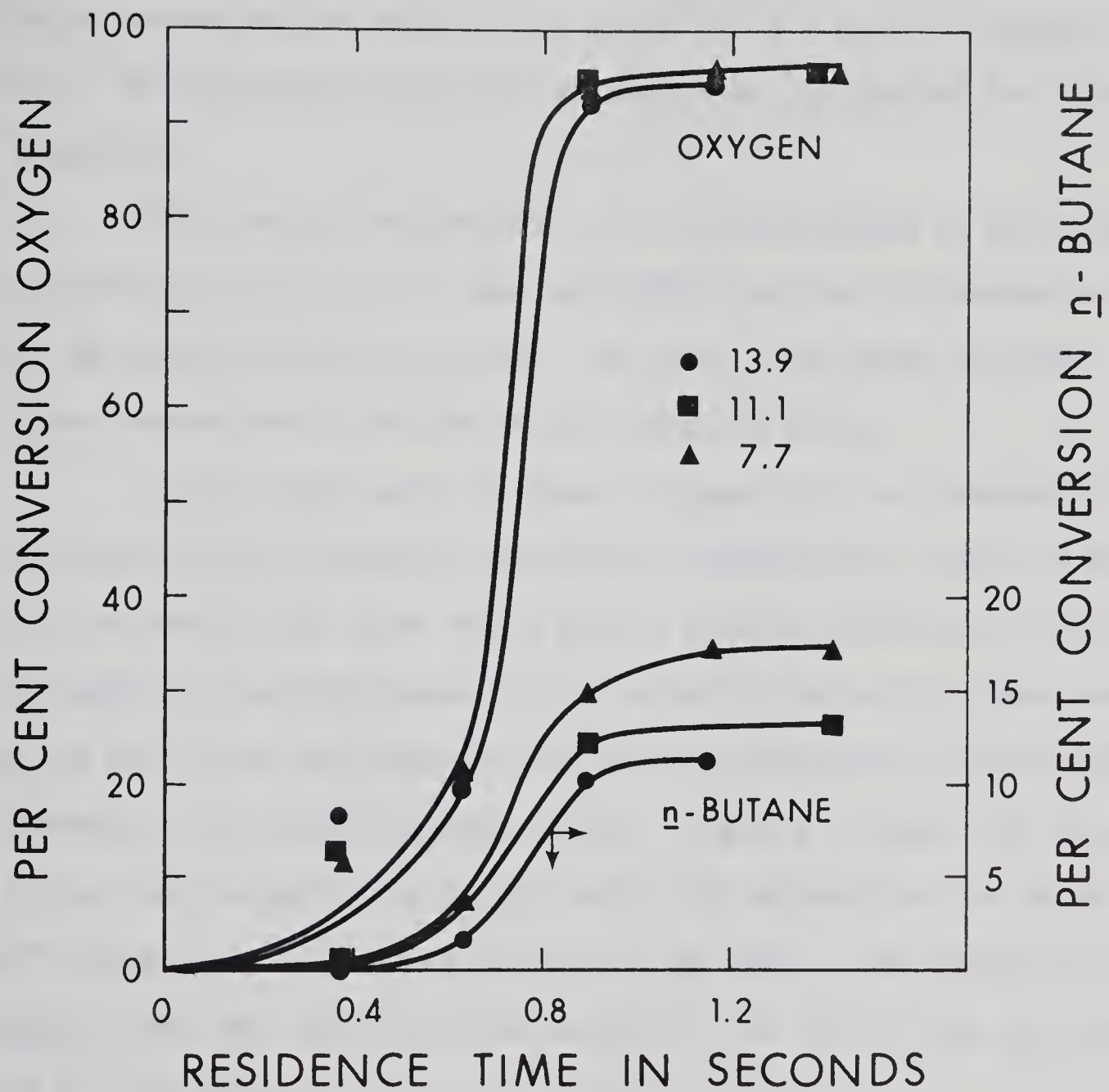


FIGURE 6.4 OVERALL CONVERSIONS - EFFECT OF INLET MOLAR RATIO

The reaction variables considered in this investigation are the starting temperatures and the starting n-butane to oxygen ratios. The starting temperatures investigated were 687°F, 702°F and 708°F, the run numbers being 65, 63 and 66, respectively. Runs 60, 61, 62, and 64 were carried out at inlet ratios of 14, 11, 8.7 and 7.7, respectively. The temperature profiles for these runs are plotted in Figures 6.1 and 6.2.

The starting temperature has a profound effect on the length of the induction period, but does not affect the rise in temperature once the induction period is over. The gases reach about the same maximum temperature at the end of the induction period.

On the other hand, as shown in Figure 6.2, the hydrocarbon to oxygen ratios do not have any significant effect on the length of the induction period, but lower ratios mean a greater temperature rise in the reactor. Some differences in the induction period for these runs are not due to the difference in the ratios, but rather because of some difference in the starting temperatures. Figure 6.3 shows that to reach a 10 per cent conversion of oxygen takes 0.36 seconds for the run at 687°F compared to 0.2 seconds for the run at 708°F. The period of rapid reaction lasts for about the same length of time for all the runs, about 0.15 to 0.20 seconds.

The overall conversion of oxygen is almost constant at around 95 per cent for all the runs. The conversion of n-butane depends upon the hydrocarbon to oxygen ratios, as shown in Figure 6.4. The conversion is lower for higher ratios. At a hydrocarbon to oxygen ratio of 14, the conversion of n-butane is approximately 13 per cent, while it is around 20 per cent at a ratio of 7.7. The higher conversion of n-butane is due

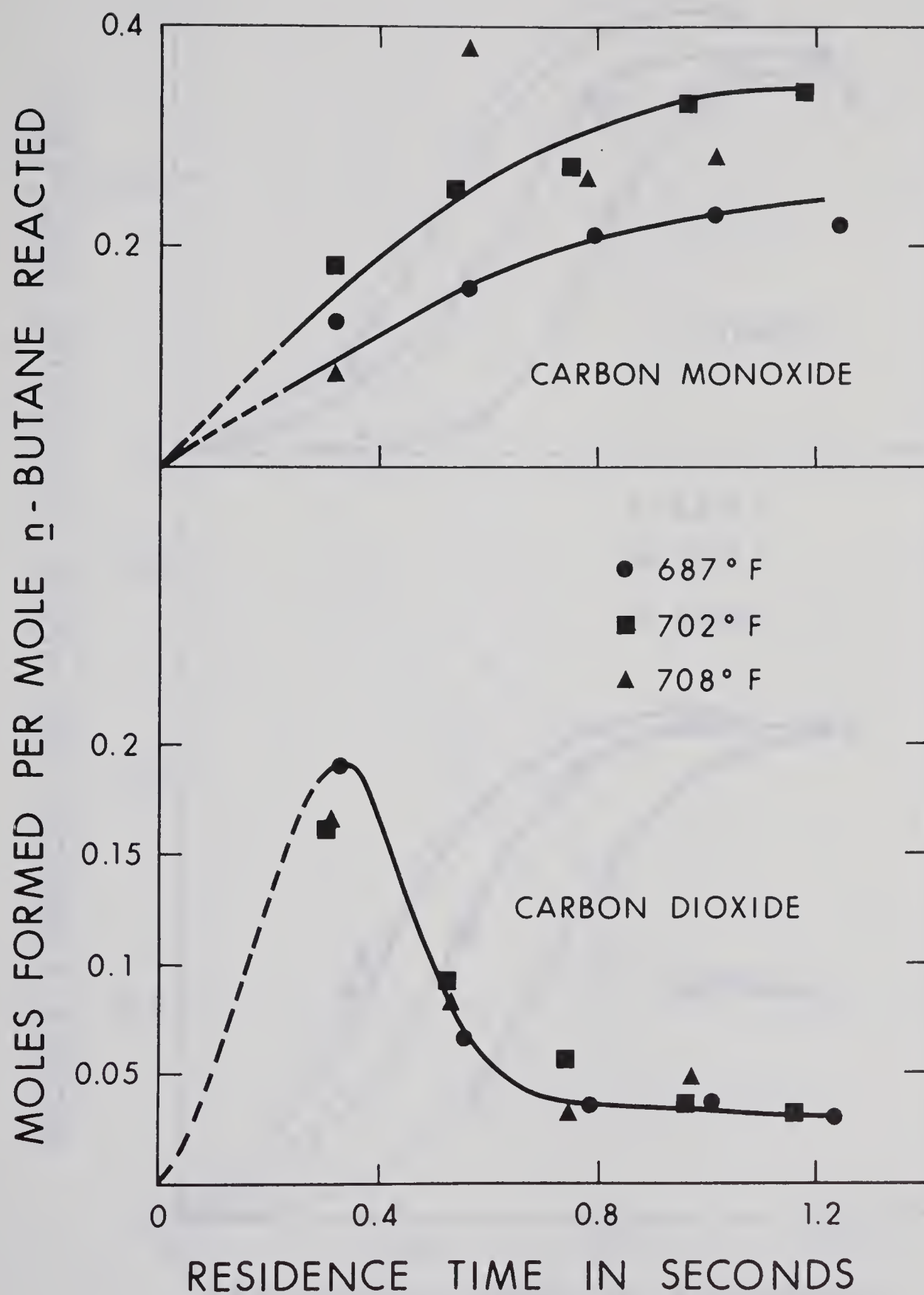


FIGURE 6.5 SELECTIVITY OF CARBON MONOXIDE AND CARBON DIOXIDE - EFFECT OF INLET TEMPERATURE

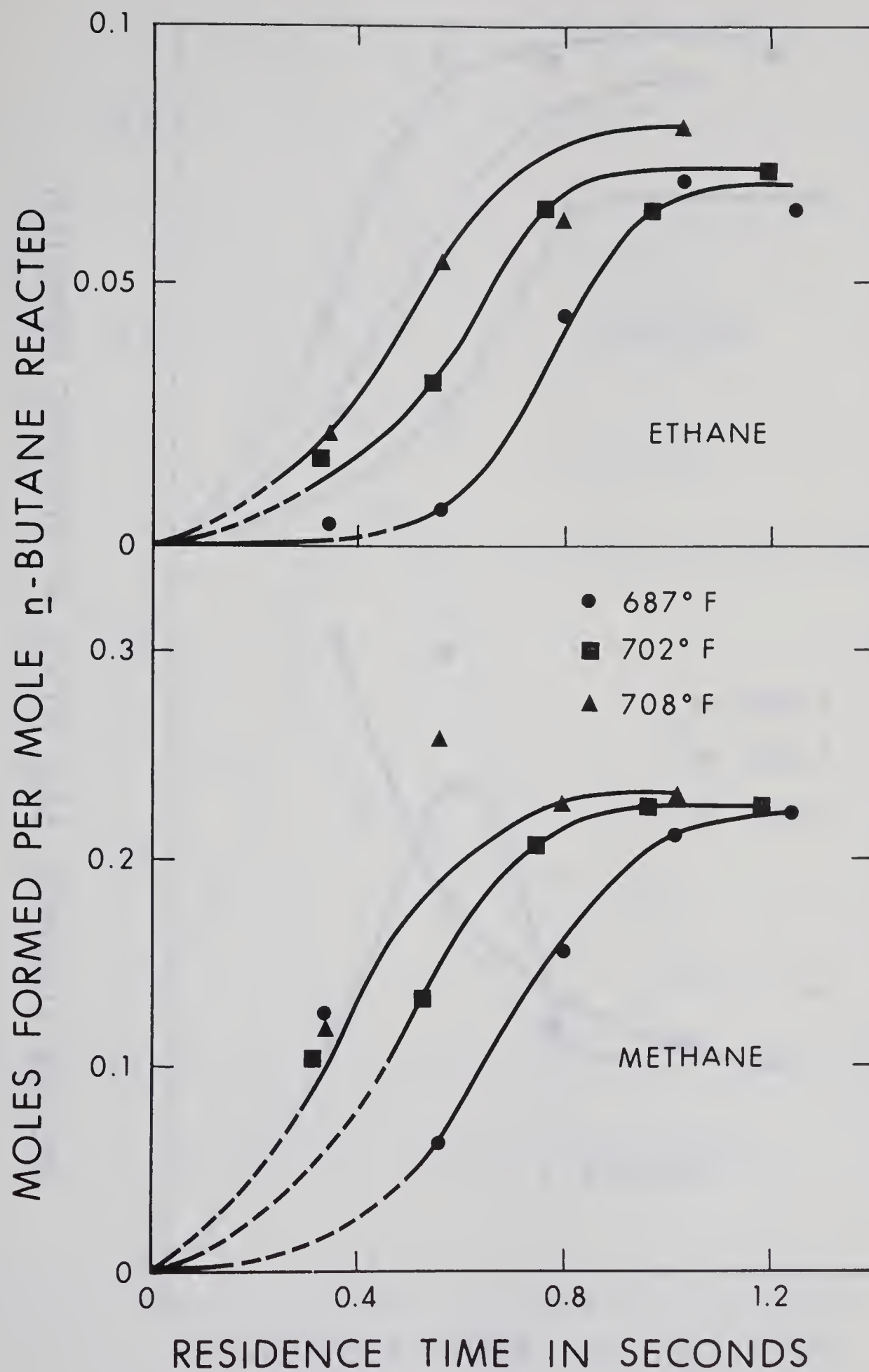


FIGURE 6.6 SELECTIVITY OF METHANE AND ETHANE-EFFECT OF INLET TEMPERATURE

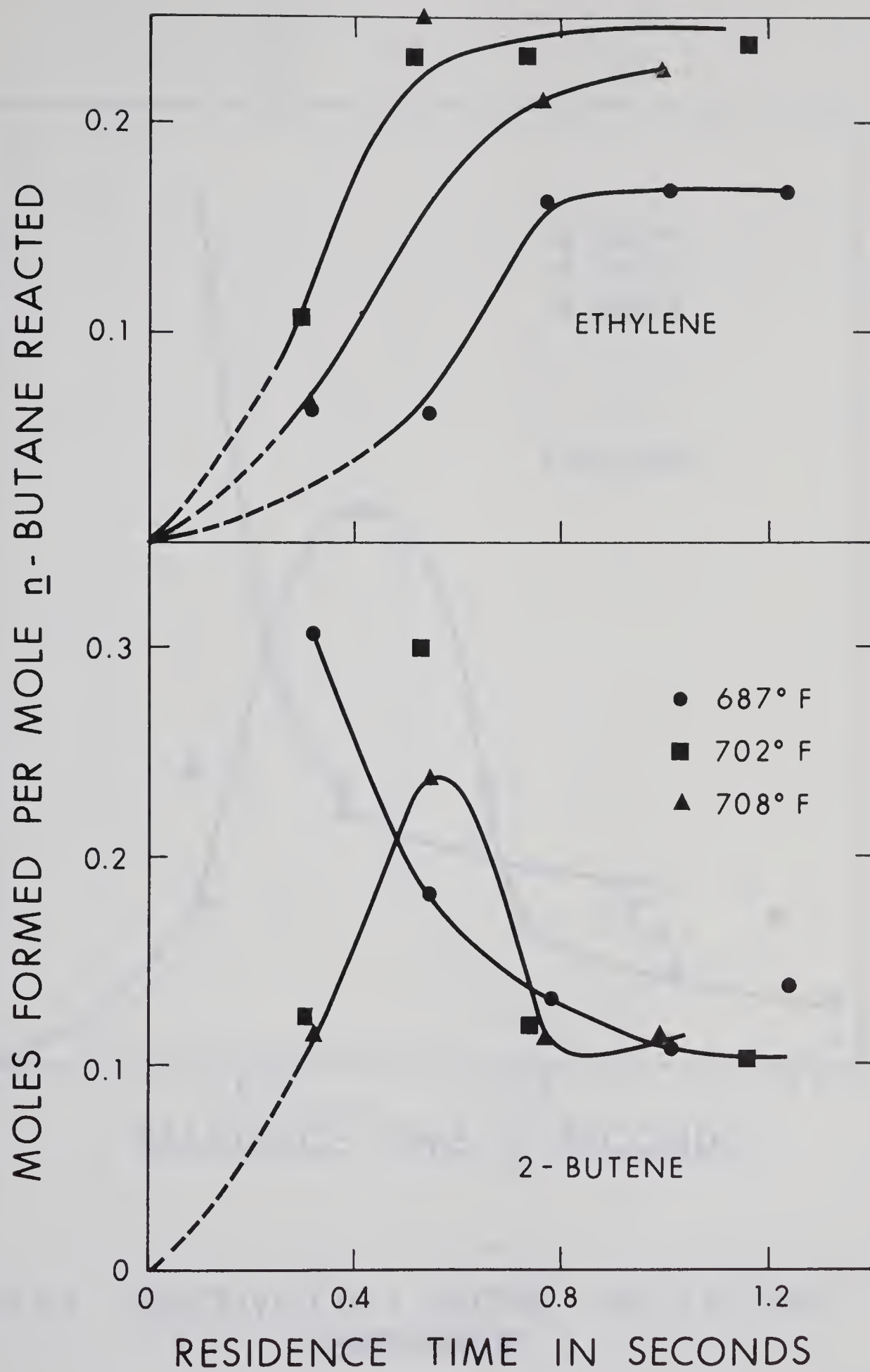


FIGURE 6.7 SELECTIVITY OF ETHYLENE AND 2 - BUTENE -EFFECT OF INLET TEMPERATURE

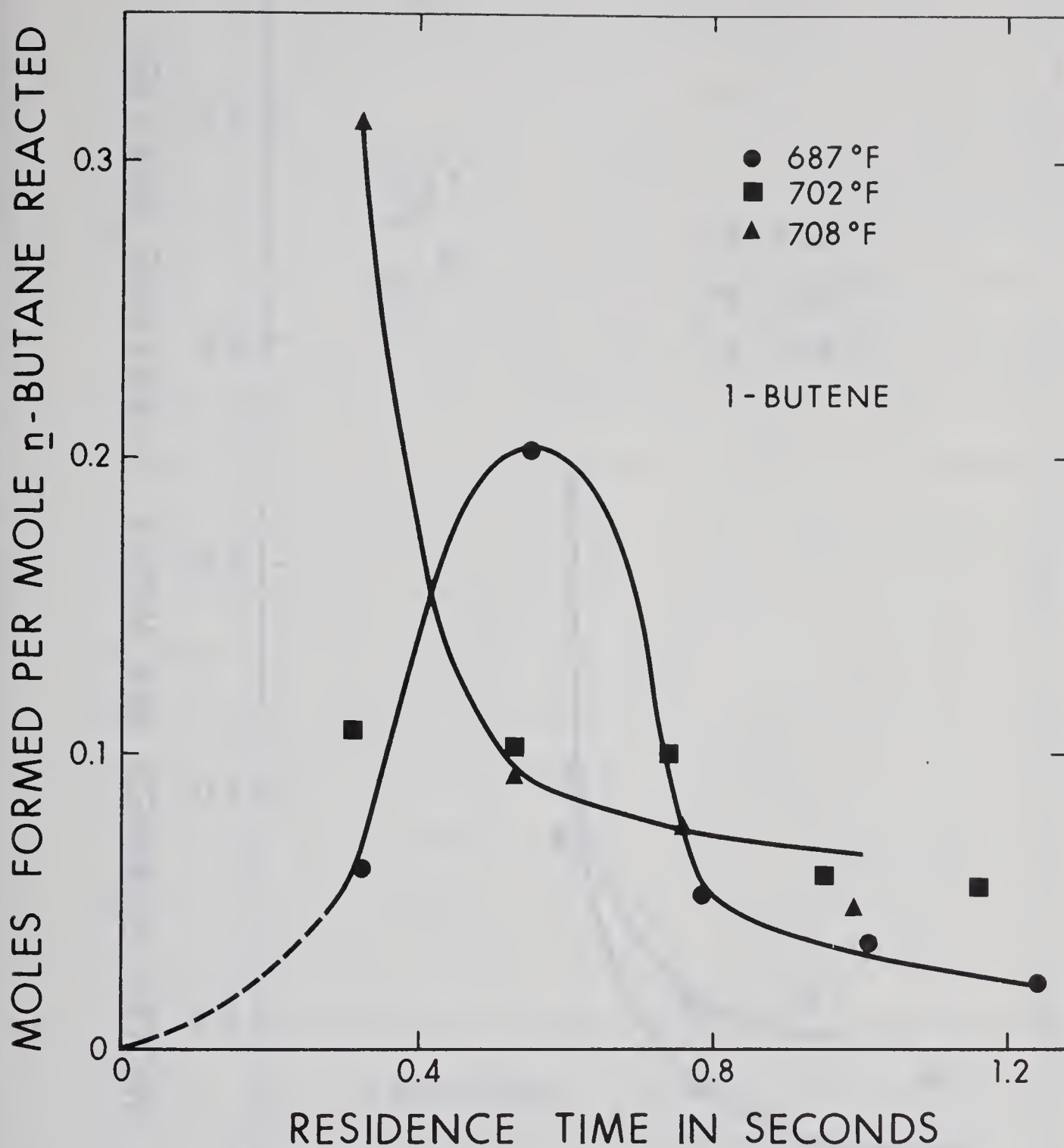


FIGURE 6.8 SELECTIVITY OF 1 - BUTENE - EFFECT OF INLET TEMPERATURE

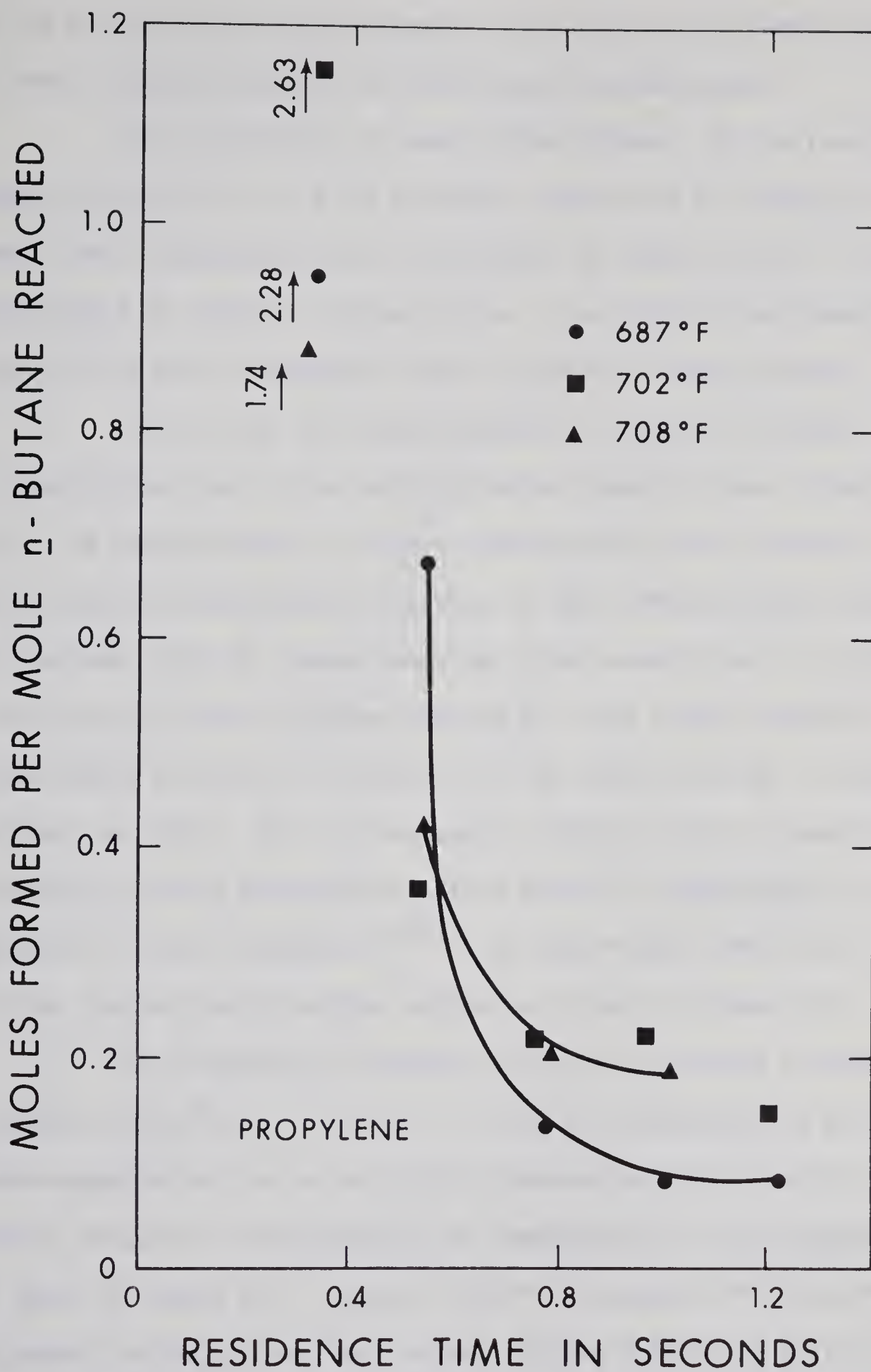


FIGURE 6.9 SELECTIVITY OF PROPYLENE - EFFECT OF INLET TEMPERATURE

to the availability of more oxygen in the system, but partly may be due to some cracking reactions at the elevated temperatures.

The distribution of some of the products of the reaction are shown in Figures 6.5 to 6.19 inclusive, depicting the effects of residence times, temperatures and hydrocarbon to oxygen ratios. All results are plotted as yield vs residence time. The yield of any component is expressed as moles component formed per mole n-butane reacted.

For any run, the carbon monoxide formation increases with residence times, while the carbon dioxide formation goes through a maximum. The larger amount of carbon dioxide during the induction period may be due to heterogeneous reaction at the surface of the reactor⁽⁴⁹⁾. The maximum yield of carbon monoxide at the reactor exit is 0.25 and 0.35 lb-mole/lb-mole n-butane reacted for runs at 687 and 702°F, respectively as shown in Figure 6.5. The carbon dioxide is almost constant at 0.027. Thus an increase in CO/CO₂ ratio is obtained at increased starting temperature. This effect of temperature has also been observed by other researchers⁽⁵⁰⁾. No significant effect was discernible for the hydrocarbon to oxygen ratios, as shown in Figure 6.13.

The formation of hydrogen, methane and ethane increased with residence times for all the runs. These were dependent on the initial temperature in so far as the initial temperature distribution is concerned, because of the influence of temperature on the induction period, as shown in Figure 6.6. However, the final amounts of these products were dependent on the hydrocarbon ratios. Figure 6.14 shows that the methane concentrations at the reactor exit are 0.22 and 0.10 for ratios of 7.7 and 13.9, respectively. The corresponding figures for ethane are 0.07 and 0.04.

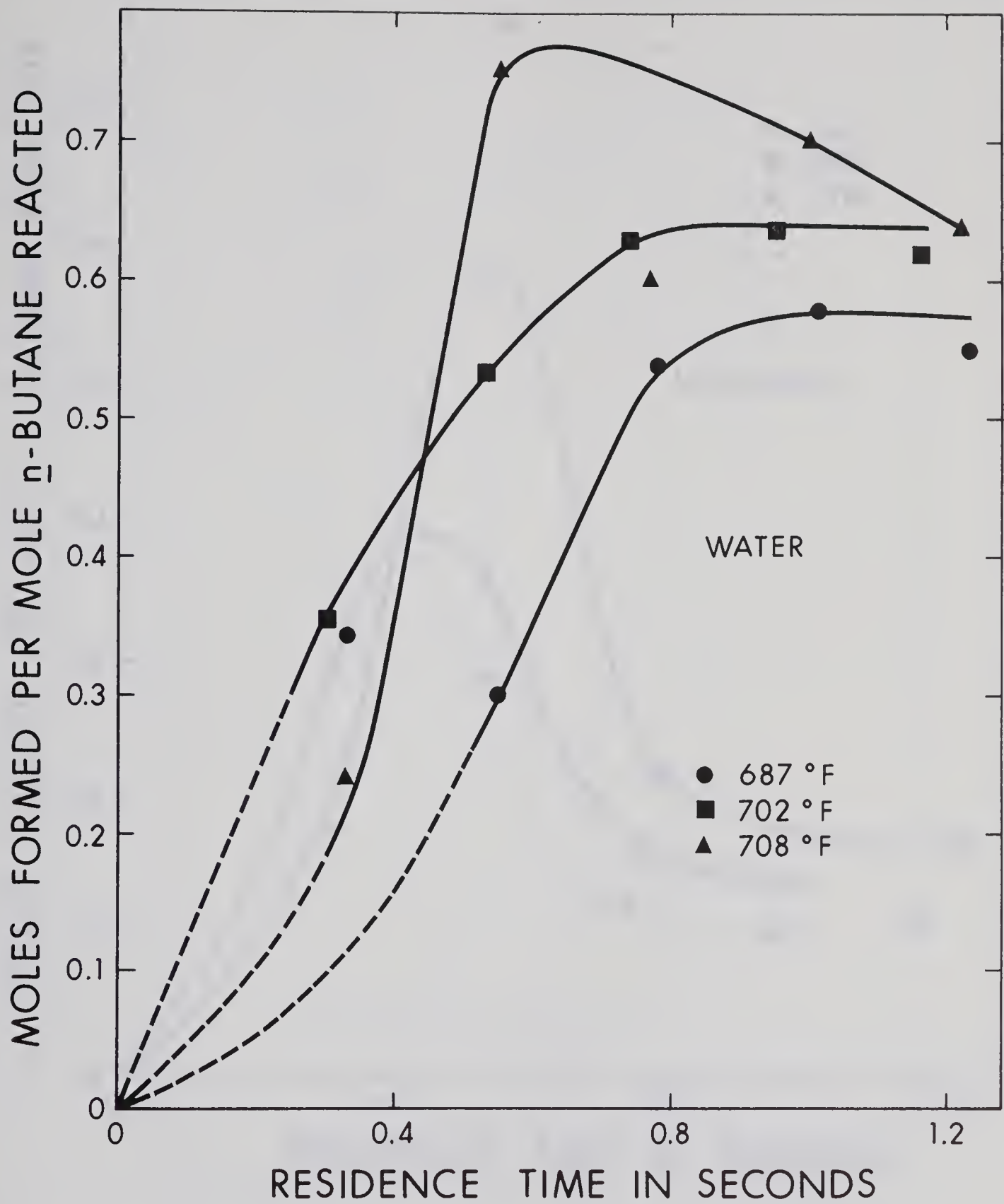


FIGURE 6.10 SELECTIVITY OF WATER - EFFECT OF INLET TEMPERATURE

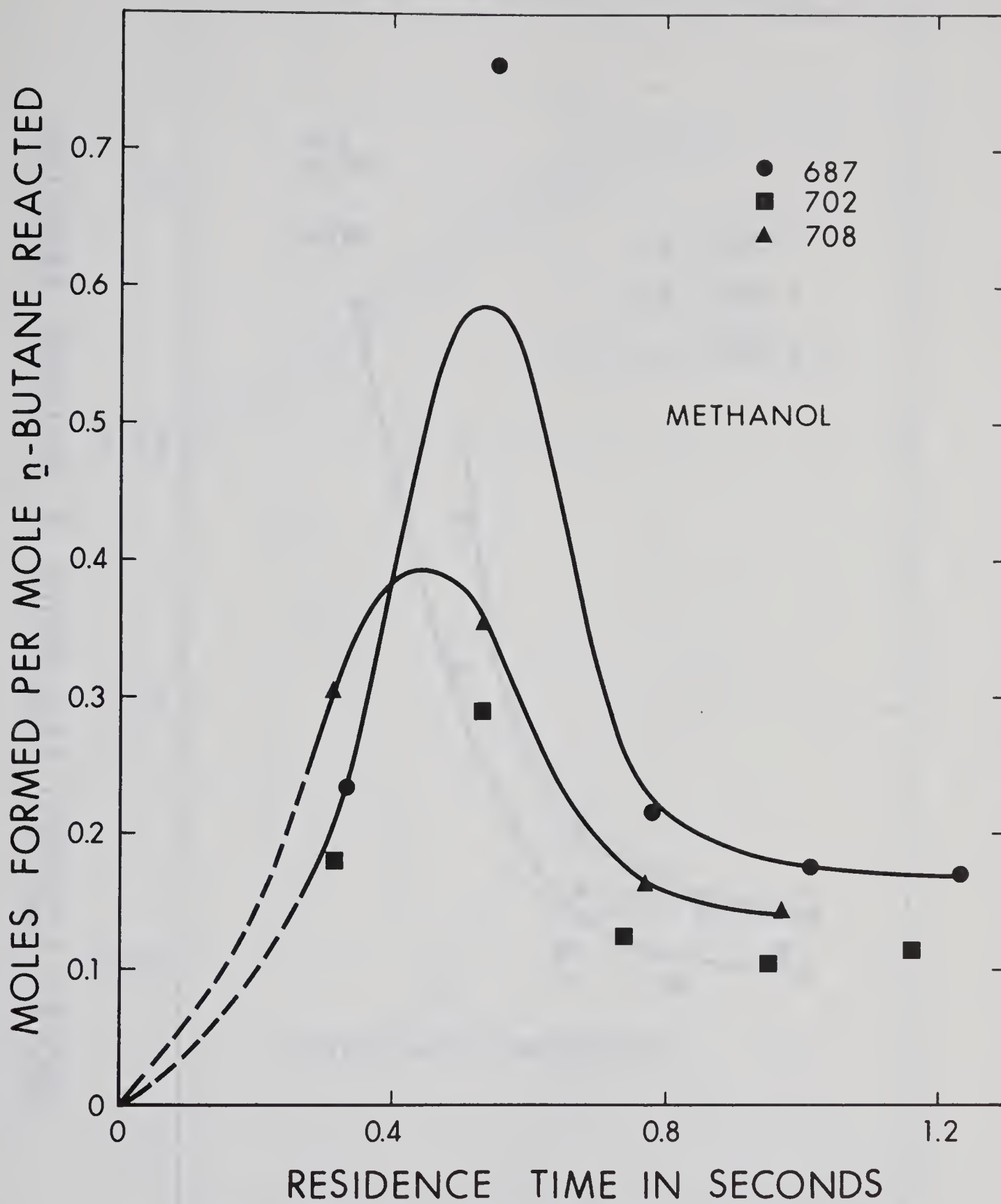


FIGURE 6.11 SELECTIVITY OF METHANOL - EFFECT OF INLET TEMPERATURE

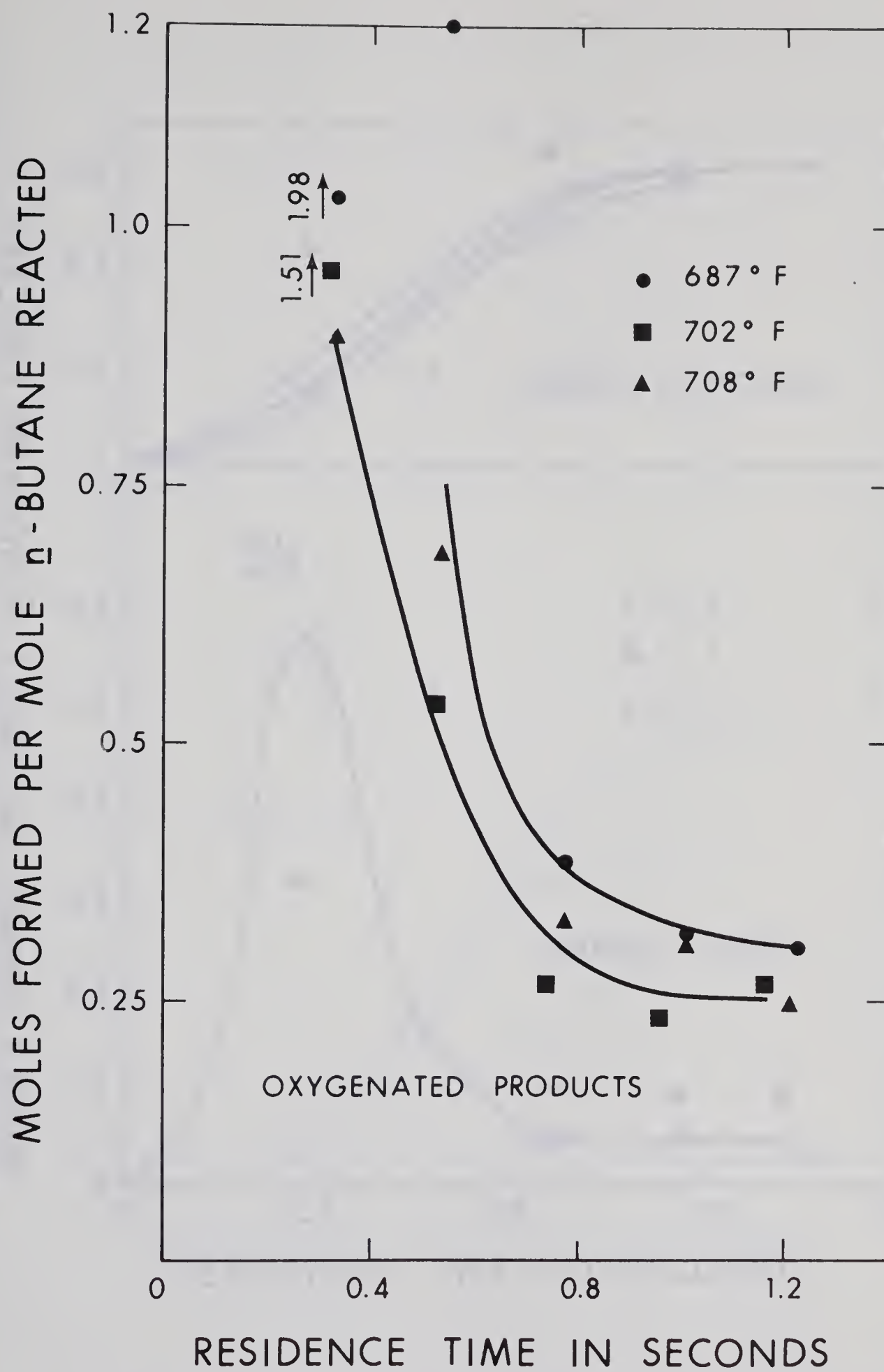


FIGURE 6.12 SELECTIVITY OF OXYGENATED PRODUCTS - EFFECT OF INLET TEMPERATURE

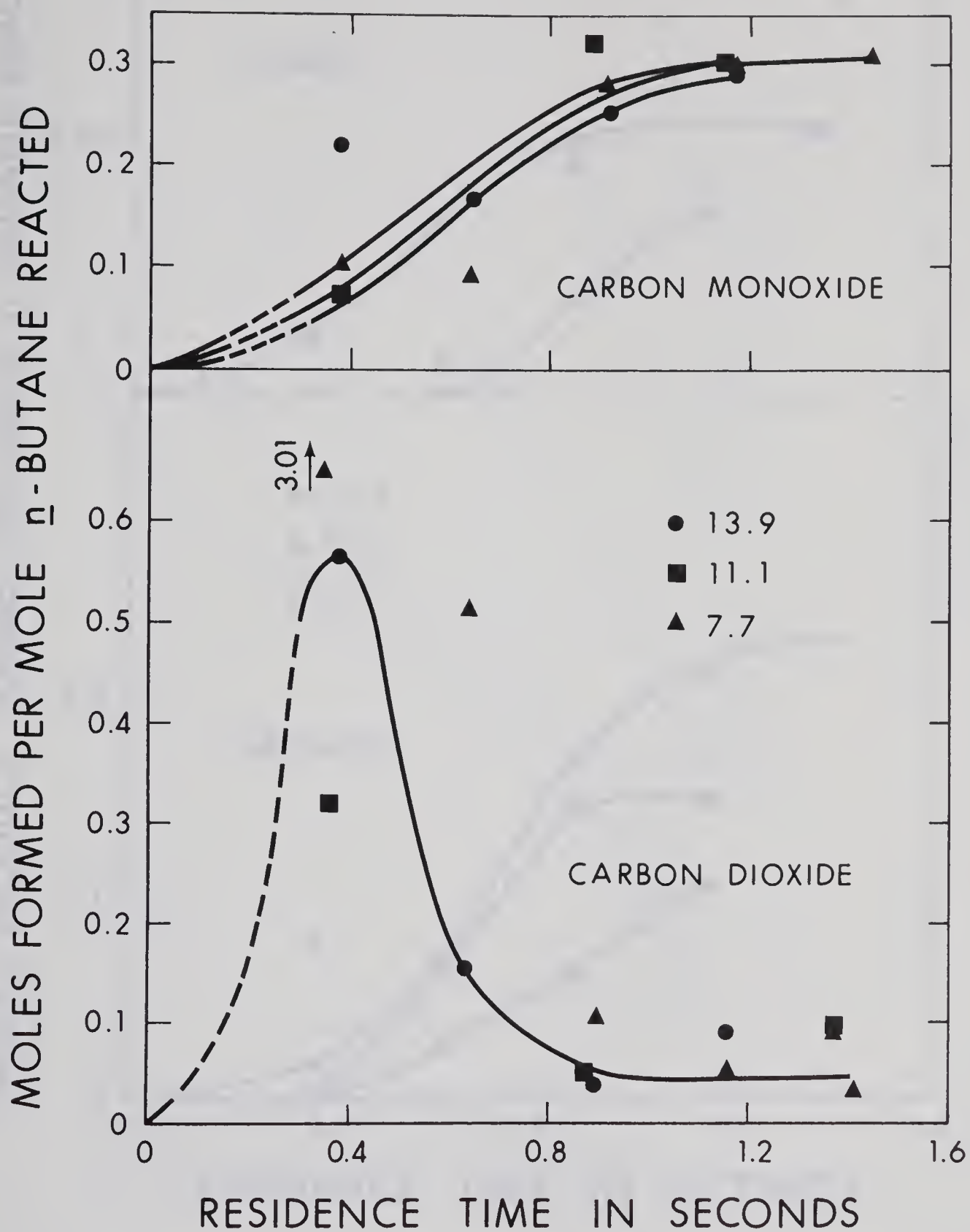


FIGURE 6.13 SELECTIVITY OF CARBON MONOXIDE AND CARBON DIOXIDE - EFFECT OF INLET MOLAR RATIO

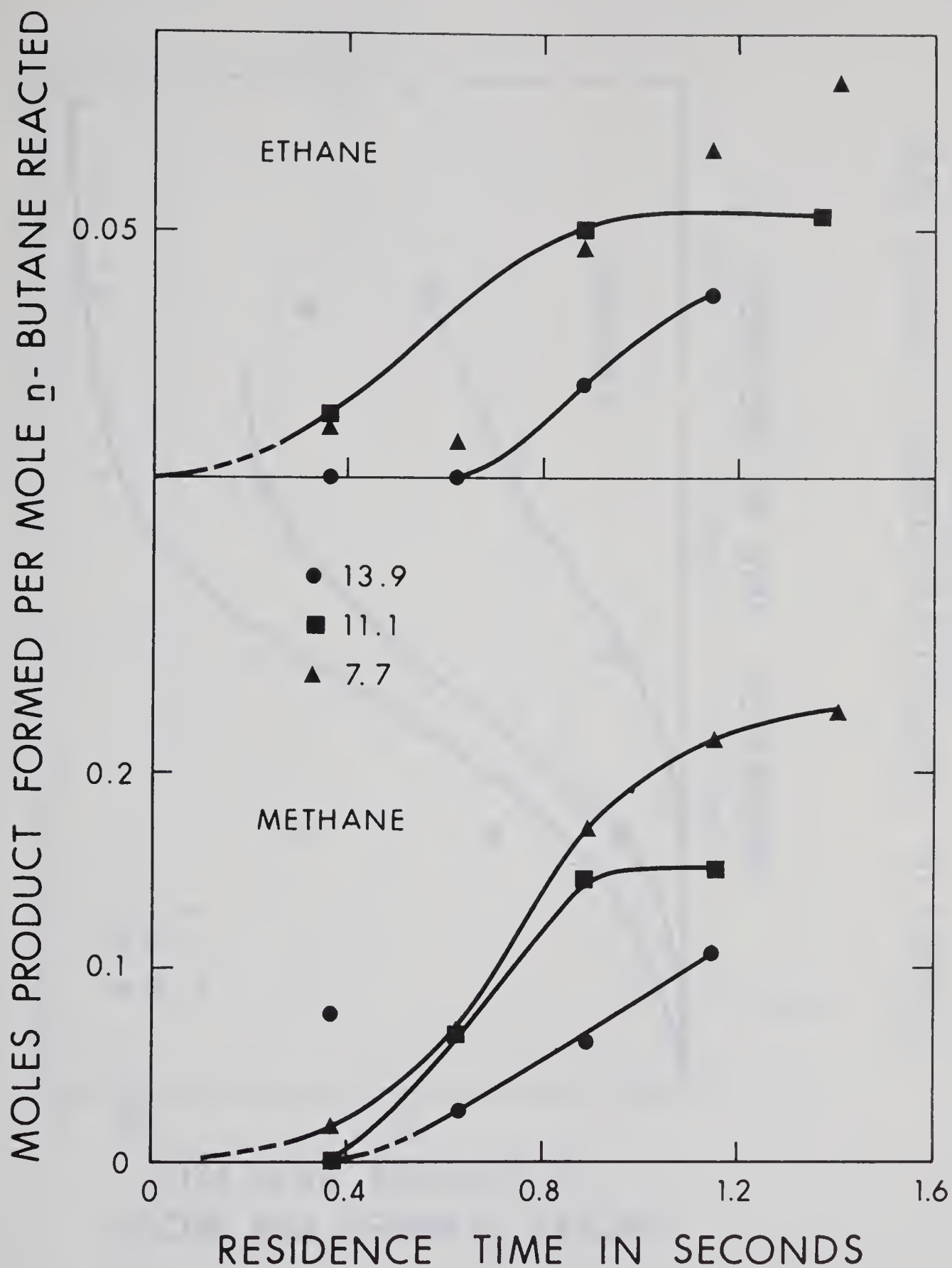


FIGURE 6.14 SELECTIVITY OF METHANE AND ETHANE - EFFECT OF INLET MOLAR RATIO

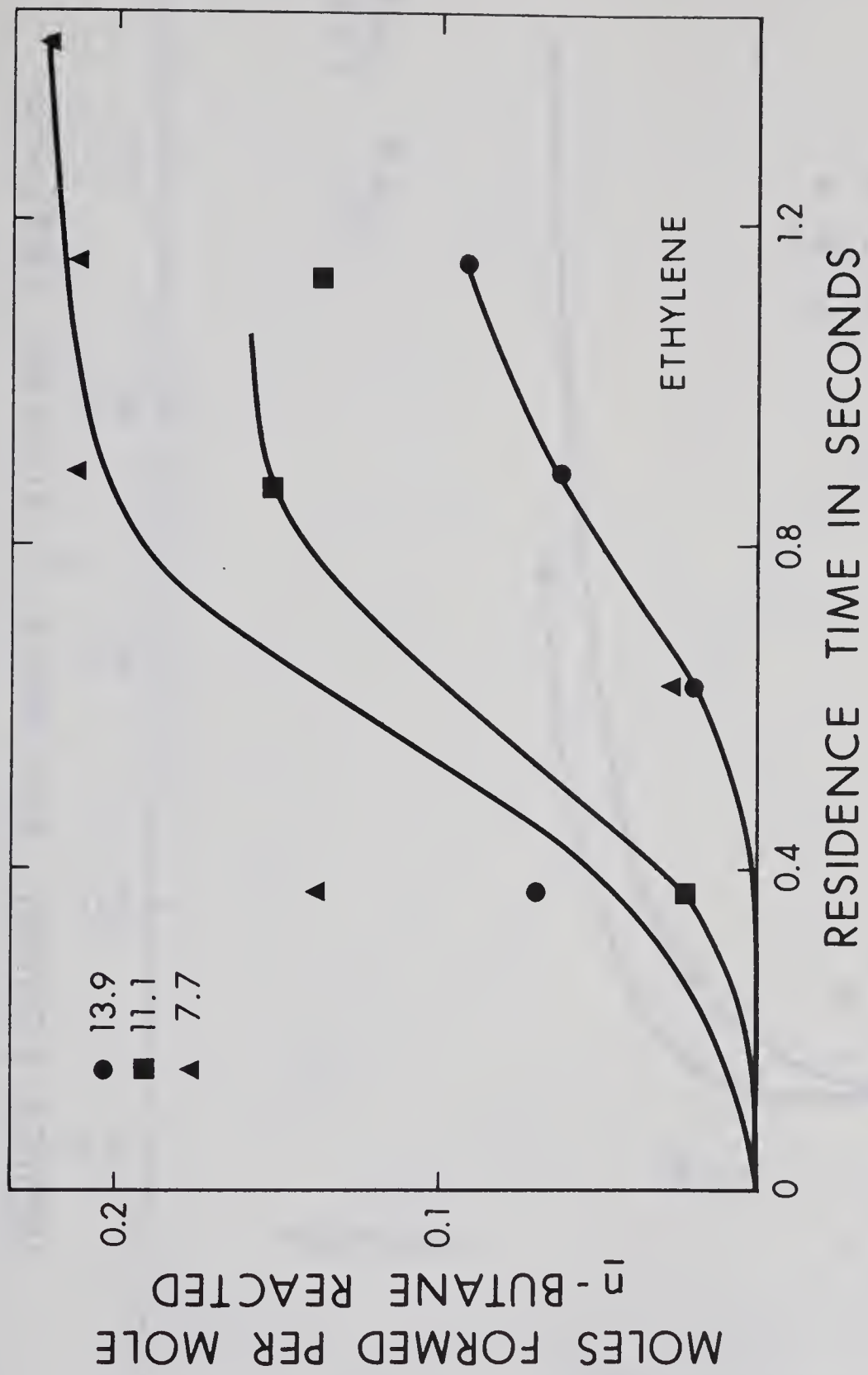


FIGURE 6.15 SELECTIVITY OF ETHYLENE - EFFECT OF INLET MOLAR RATIO

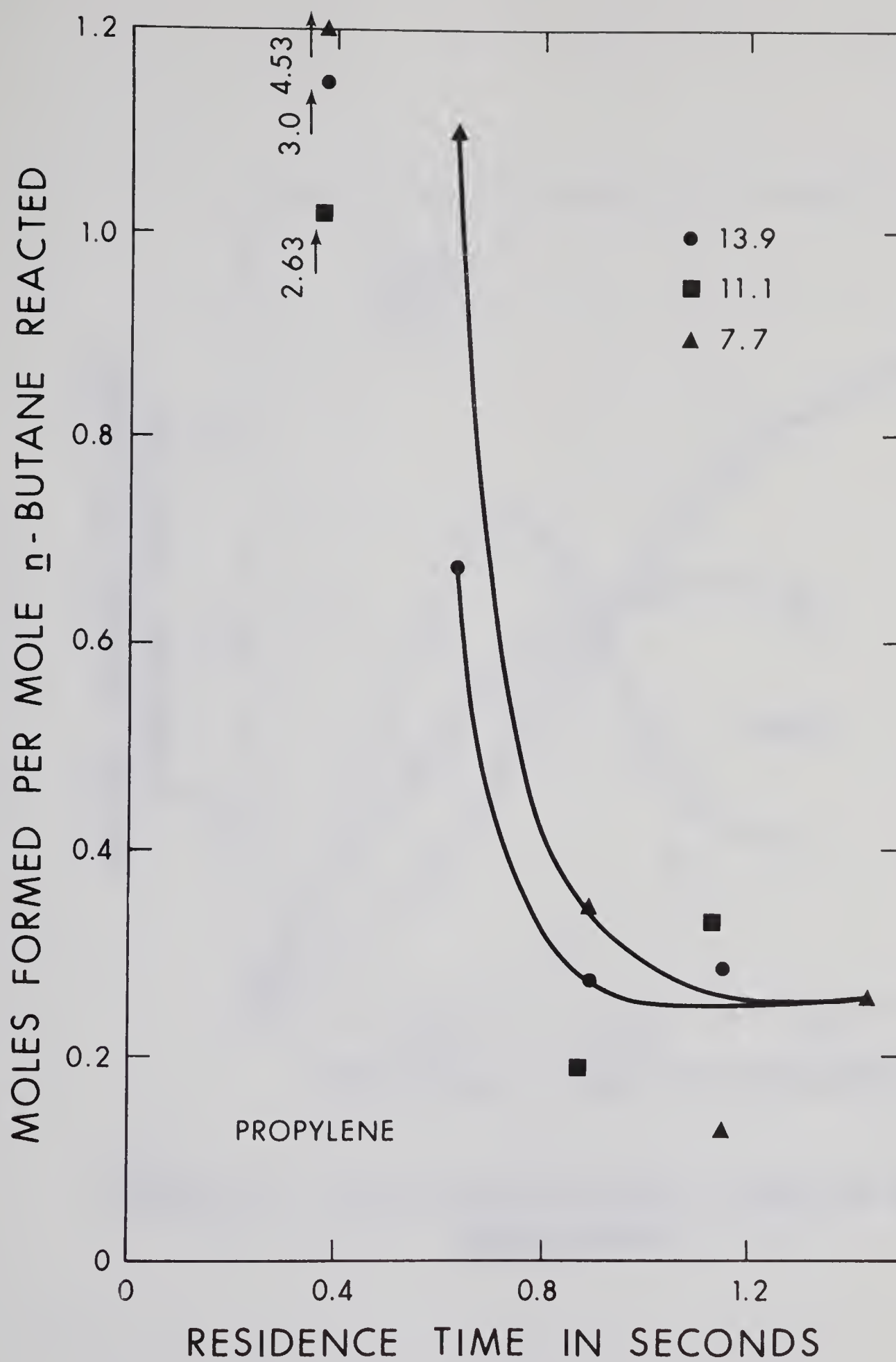


FIGURE 6.16 SELECTIVITY OF PROPYLENE - EFFECT OF MOLAR RATIO

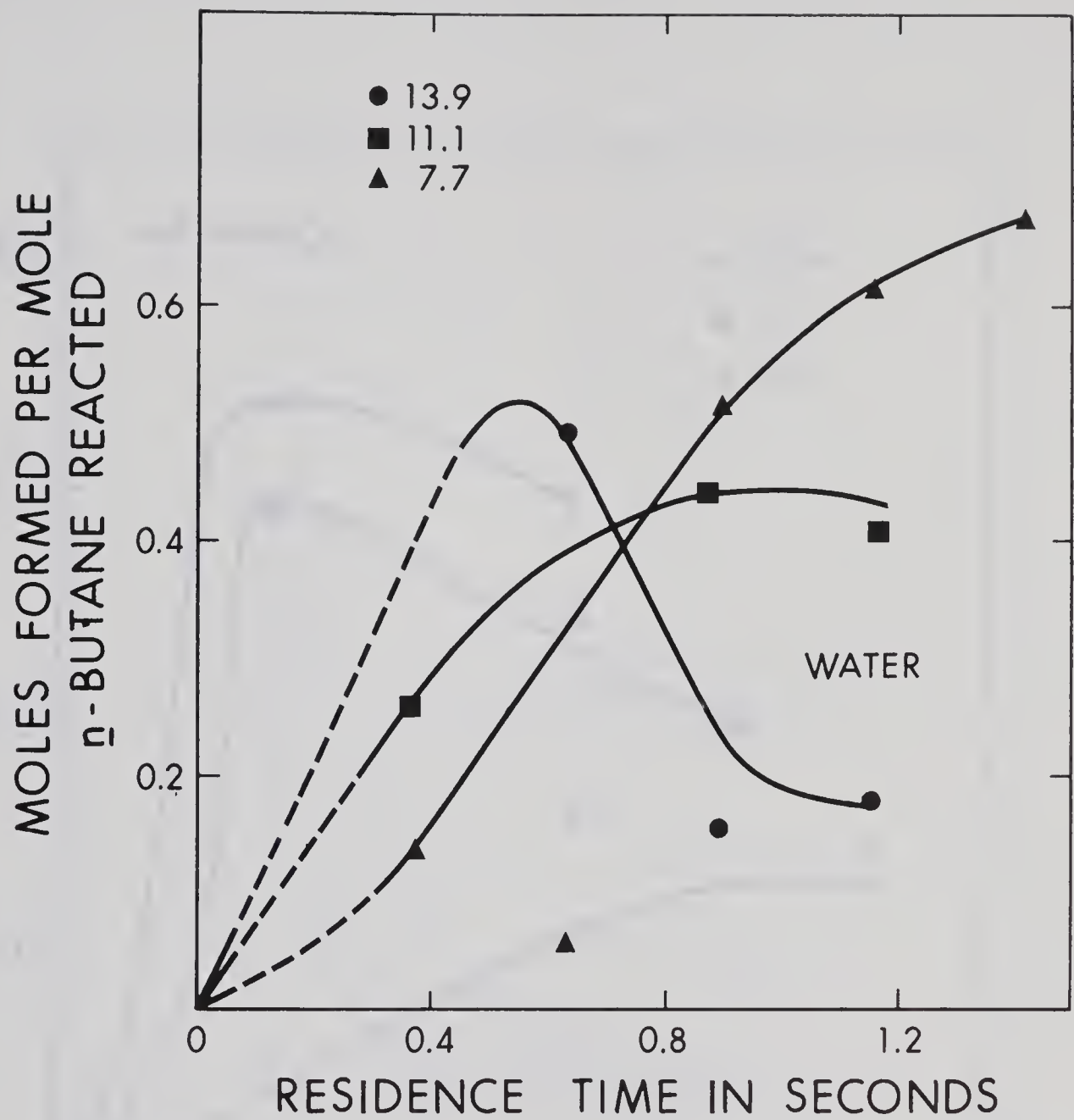


FIGURE 6.17 SELECTIVITY OF WATER - EFFECT OF INLET MOLAR RATIO

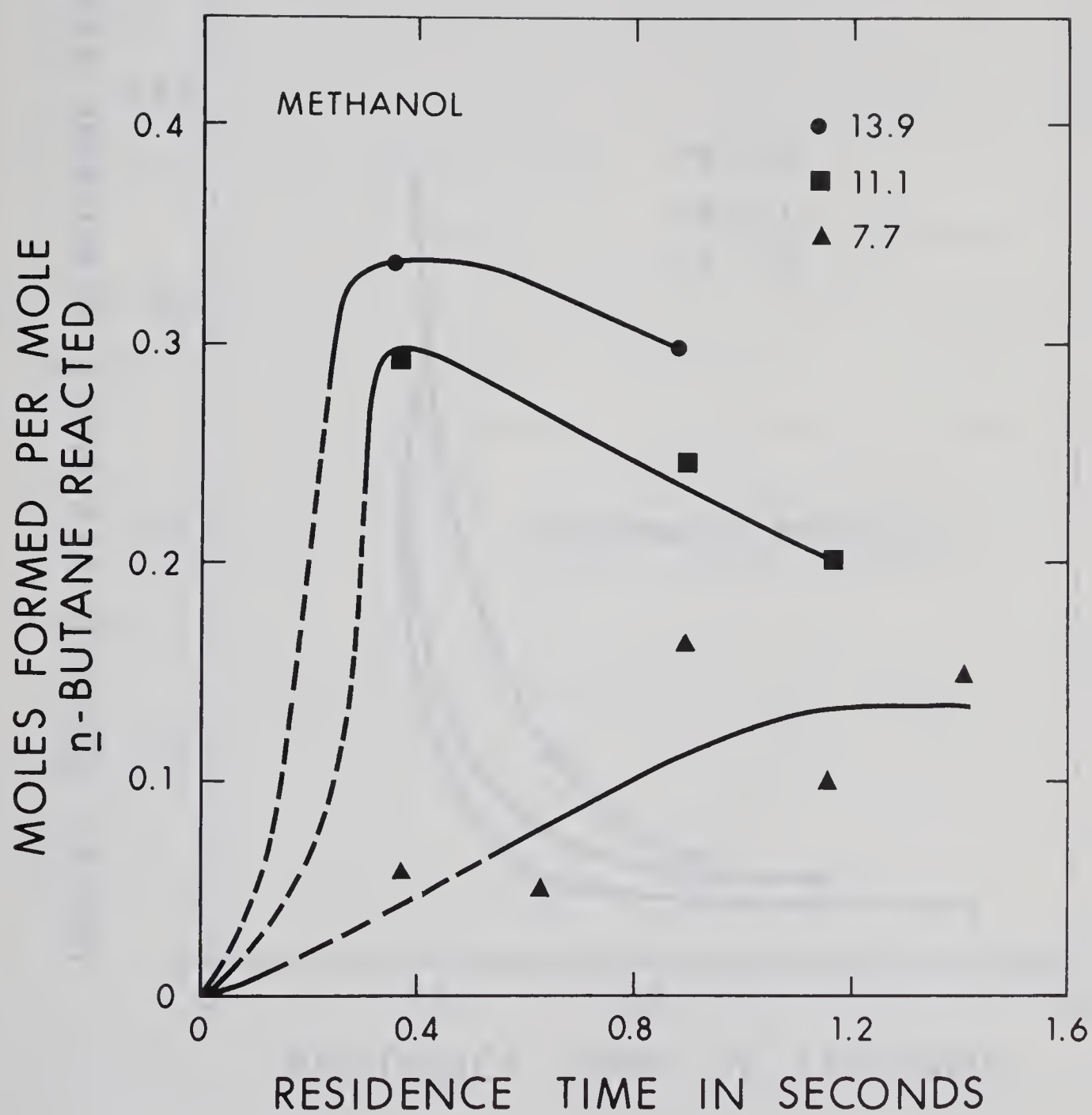


FIGURE 6.18 SELECTIVITY OF METHANOL - EFFECT OF MOLAR RATIO

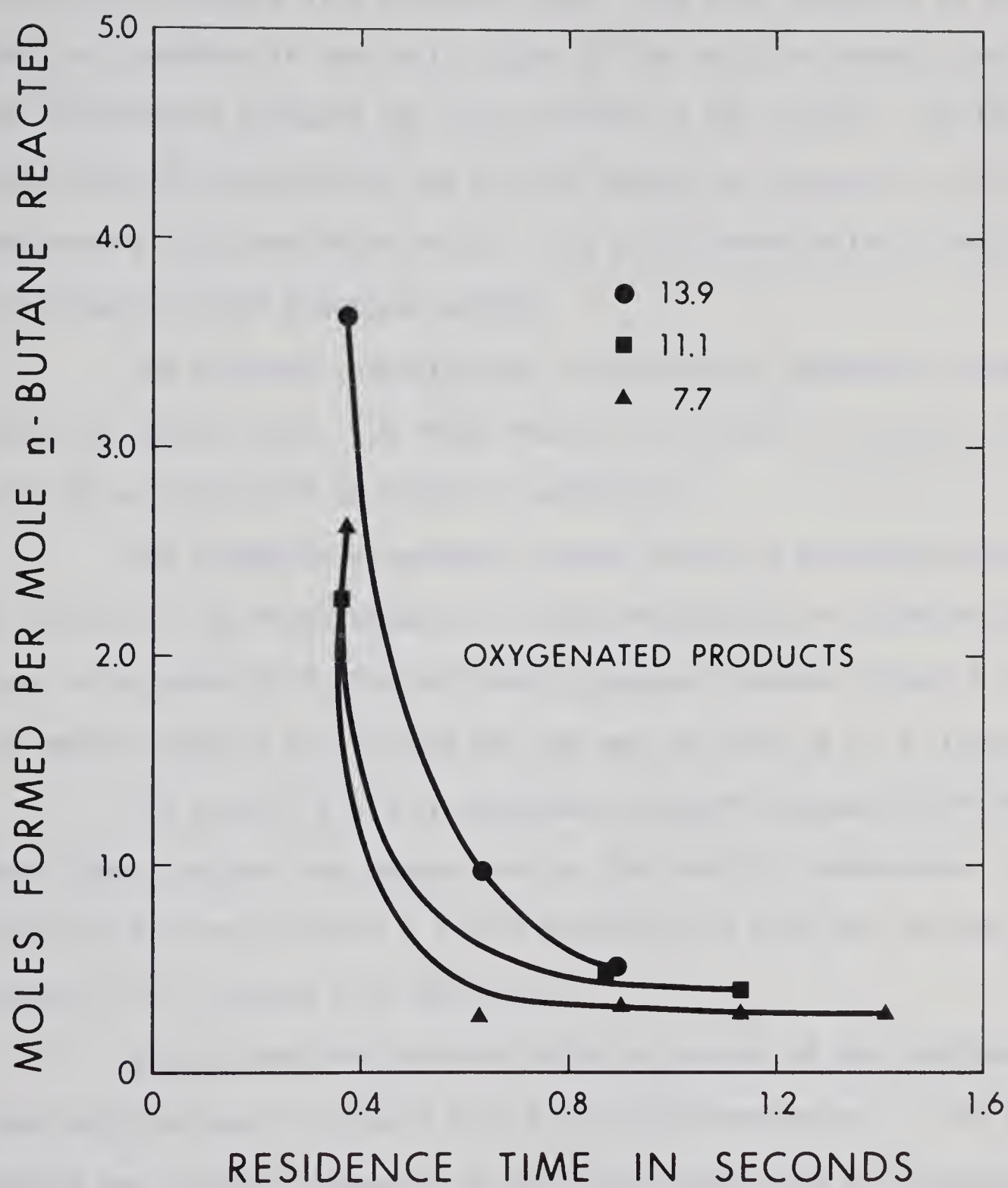


FIGURE 6.19 SELECTIVITY OF OXYGENATED PRODUCTS - EFFECT OF INLET MOLAR RATIO

Figures 6.7 to 6.9 and 6.15 and 6.16 show the olefin formation for different runs. The olefin formation except ethylene which increases, decreases with residence time. The high formation of propylene and n-butenes in the early stages of the reaction suggest that these are intermediate products and react further in the reactor. No definite trend could be observed for the olefins because of change in starting temperature and hydrocarbon ratios. The exit concentration is about 0.3 lb-mole/lb-mole n-butane reacted.

The ethylene concentration is affected by temperature and hydrocarbon to oxygen ratio. It rises from 0.175 at 687°F to 0.225 at 708°F, and 0.08 at ratio 13.9 to 0.225 at ratio 7.7.

The formation of methanol passed through a maximum for most of the runs. The final amount is little affected by the starting temperature, being about 0.15 lb-mole/lb-mole n-butane reacted (Figure 6.11). The amount rises to 0.3 lb-mole for the run at ratio of 13.9 (Figure 6.18).

The overall yield of oxygenated products decreases with residence time, and does not depend much on the starting temperature. The yield for the run at ratio 7.7 is 0.3 while it is 0.43 for the run at ratio of 13.9 (Figures 6.12 and 6.19).

Water formation increased with the extent of the reaction, reaching a maximum of about 0.6 to 0.65 at the reactor exit. The concentration was slightly dependent on the inlet temperature and hydrocarbon ratio (6.10 and 6.17). The decrease in water for the run at ratio 13.9 may be due to poor water analysis.

The large increase in temperature during the progress of the reaction makes interpretation of the plots very difficult, both because of the complicating effect of the temperature on the course of the reaction

and because of the increased sensitivity of the different quantities in the figures to small changes in the abscissa. For this reason, it was intended to observe the reaction at lower conversion when the rise in temperature was small. This was done for runs 60, 61 and 64 using the Figures 6.2, 6.4 and 6.19, using a residence of 0.65 seconds which is before the steep part of the temperature profile.

Table 6.3 shows the amount of oxygenated products and the conversions of n-butane at a residence time of 0.65 for runs 60, 61 and 64.

TABLE 6.3

Run No.	Oxygenated Compounds	Conversion of <u>n</u> -Butane
60	0.87	2.0
61	0.61	3.0
64	0.36	4.5

Table 6.4 shows the residence time and oxygenated products formed at a fixed conversion of 3.5 per cent n-butane for the same runs. The maximum temperature rise for each run is also given.

TABLE 6.4

Run No.	Residence Time Sec.	Oxygenated Products	Maximum Temperature Rise °F
60	0.70	0.74	230
61	0.66	0.60	263
64	0.62	0.385	335

These results are plotted in Figures 6.20 to 6.23. Figure 6.20 shows that the conversion of n-butane is linear with the hydrocarbon to oxygen ratio, an observation similar to that obtained by Jones et al⁽²⁹⁾.

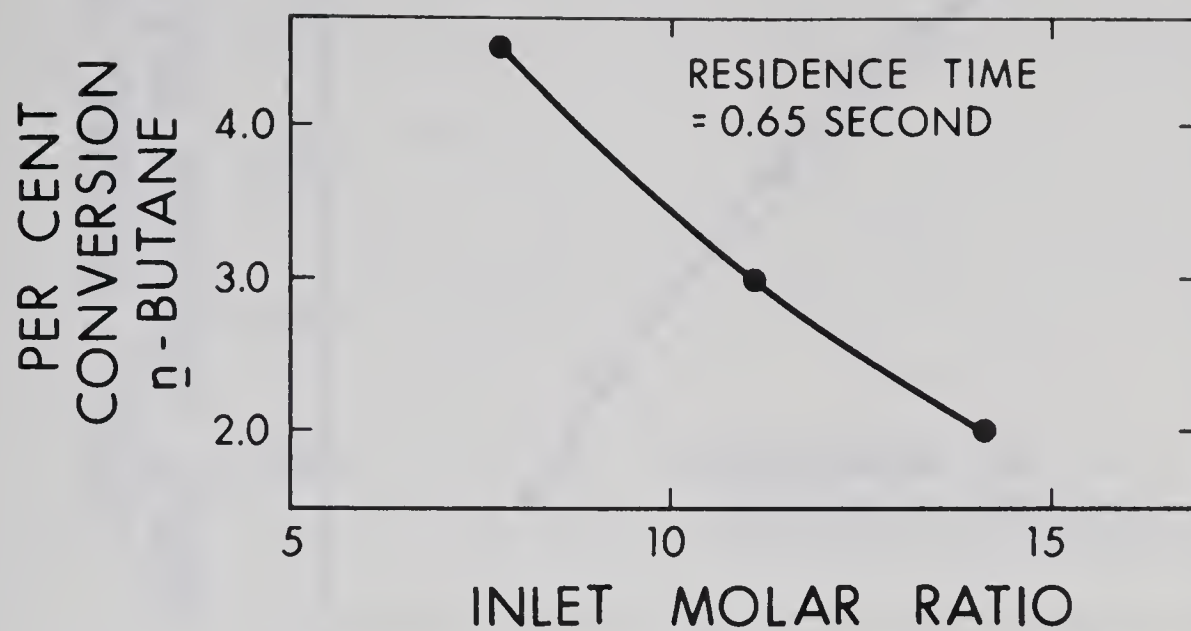


FIGURE 6.20 EFFECT ON n-BUTANE CONVERSION

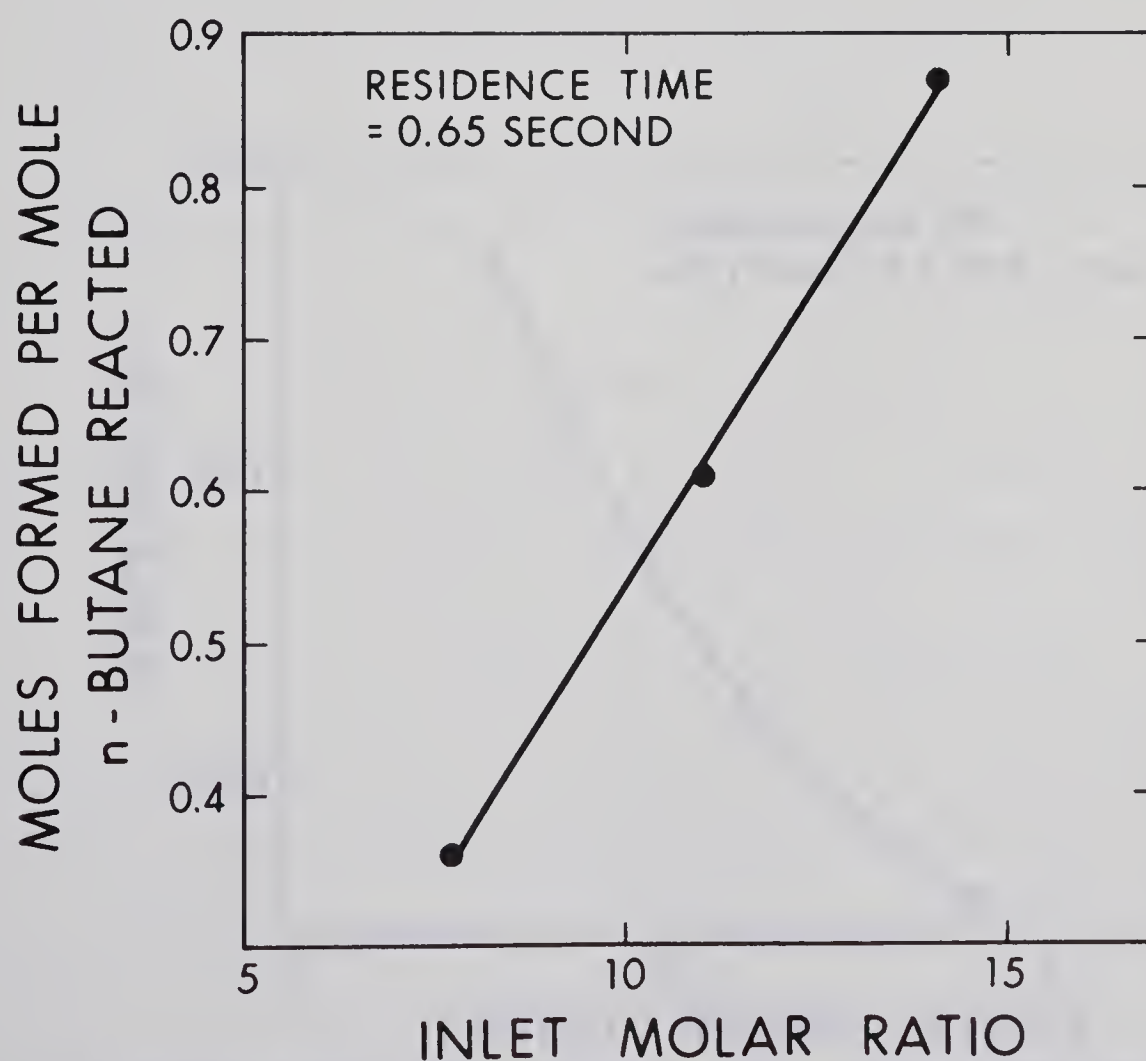


FIGURE 6.21 EFFECT ON SELECTIVITY OF OXYGENATED PRODUCTS

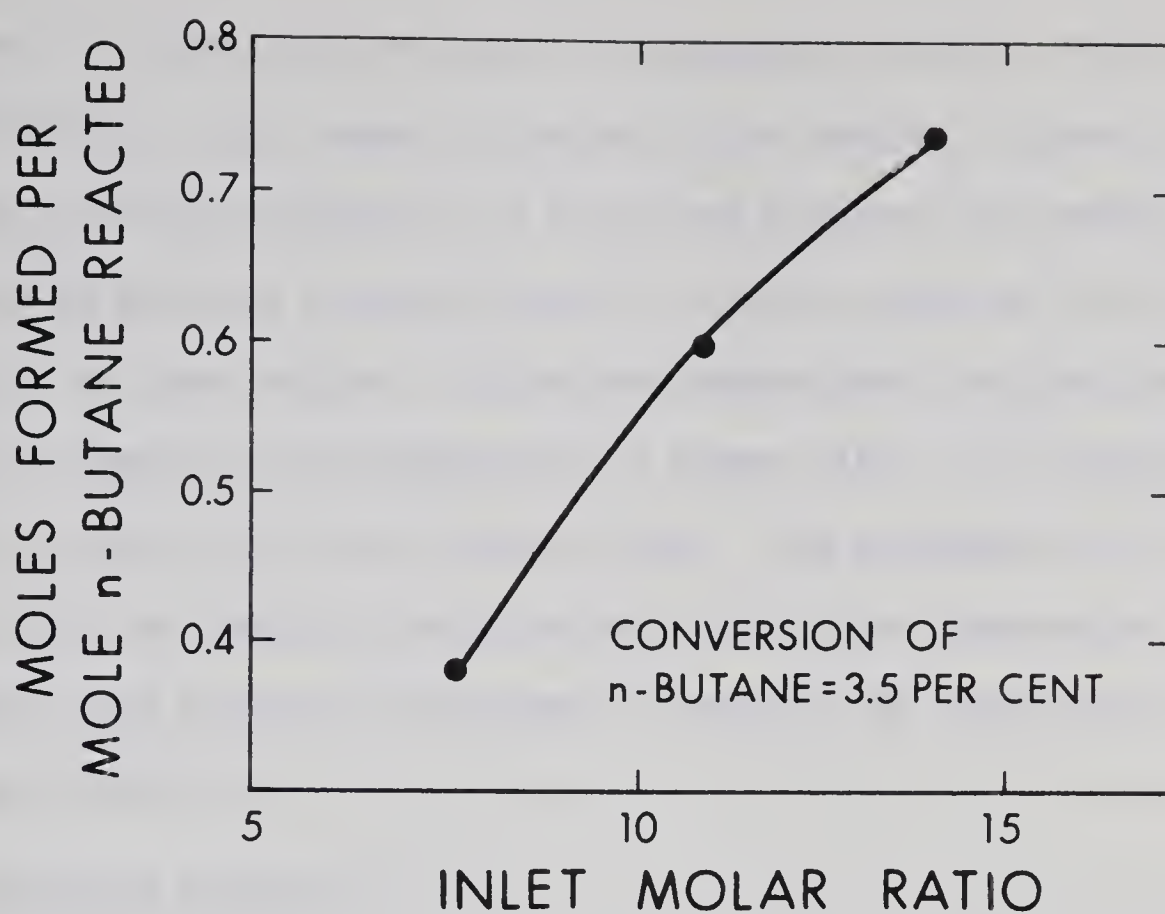


FIGURE 6.22 EFFECT ON SELECTIVITY OF OXYGENATED PRODUCTS

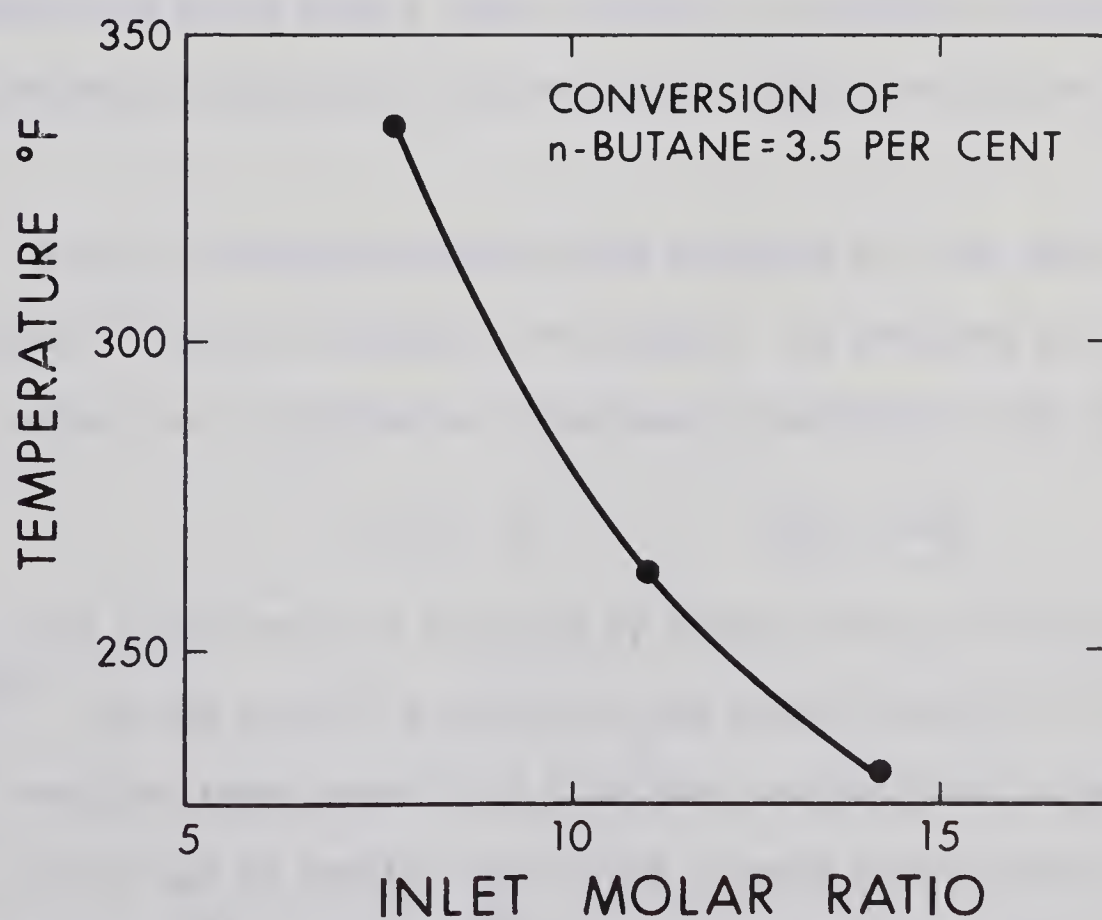


FIGURE 6.23 EFFECT ON MAXIMUM TEMPERATURE RISE

Figure 6.21 shows that the amount of oxygenated products rises sharply with decrease in the amount of oxygen in the system. Figure 6.22 shows that at a fixed conversion of 3.5 per cent n-butane, the amount of oxygenated products is much higher for a run at ratio of 13.9 compared to a run at lower ratios. The maximum temperature rise has already been noted to depend on the hydrocarbon to oxygen ratio. This dependence is shown in Figure 6.23 to be almost linear. The agreement of Figures 6.20 to 6.23 to the generally accepted behaviour of the hydrocarbon oxidation reaction lend support to the general nature of the curves drawn in Figures 6.2, 6.4 and 6.19.

6.5 Reaction Mechanism

The distribution of the products of the reaction with residence time and the effects of the operating variables on the distribution can give important clues as to the mechanism of the reaction. A knowledge of the mechanism would enable better choice of variables and other reactor parameters and would lead to better reactor design and process economy.

One very interesting mechanism proposed for the reaction is that by Knox⁽⁹⁾ for the oxidation of propane. He obtained 80% of the initial products of oxidation as propylene, according to the reaction



However, this result was not obtained by several other investigators (11,51,52). In the case of n-butane in the present study, not only butenes, but also large amounts of propylene are obtained as major initial products. This can be readily taken into account by the isomerization scheme of Semenov⁽²⁾ and Shtern⁽⁸⁾, as discussed in section 2.2. This, at the same time, explains the formation of a large amount of formaldehyde, acetaldehyde and methanol in the reaction products in the early

stages.

The larger alkoxy radicals formed in the isomerization reaction scheme would likely break up and subsequently form paraffin by reacting with n-butane. The methoxy radical, at the lower temperatures, will form methanol by abstracting a hydrogen atom from the n-butane molecule. As the temperature rises, there will likely be a competing cracking route and hence the maximum in the formation of methanol will occur. In addition, methanol itself can get oxidized at the high temperatures reached in this study. Norrish and Porter⁽⁴¹⁾ obtained appreciable secondary oxidation of methanol during the oxidation of n-butenes.

The role of aldehydes is now relatively well established. Salooza⁽⁵³⁾ found that acetaldehyde is the most reactive aldehyde and the reactivity does not increase with increase in the carbon chain length, as is the case with hydrocarbons. Formaldehyde was found to be far less reactive compared to others. However, in the present case, since the reaction condition is quite severe, all the aldehydes are likely to take part in the reaction. This is borne out by the experimental results which show a steep decrease in the amount of aldehydes at the end of the induction period.

The yield of propylene and n-butenes decrease sharply in the same pattern as aldehydes. The yield of ethylene only increases with reaction. This strongly suggests a pivotal role being played by olefins, as suggested by Knox. At the temperature of this study, ethylene does not enter into the reaction, but propylene and n-butenes may do so in accordance with the mechanism of Knox. A relatively large amount of ethylene oxide and propylene oxide found in the initial products lends further evidence to this postulate. Accordingly, a mechanism combining

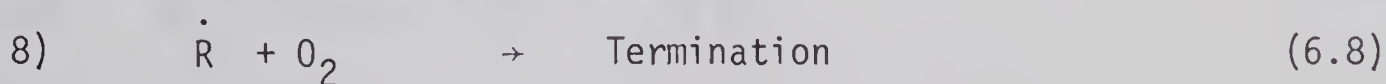
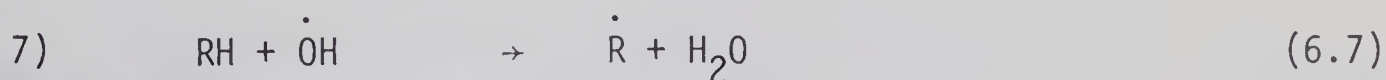
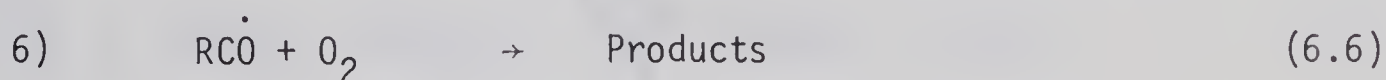
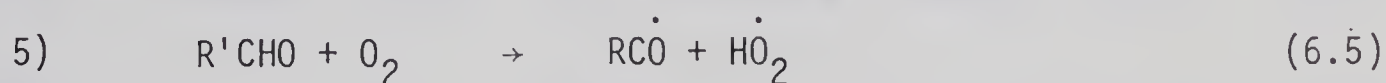
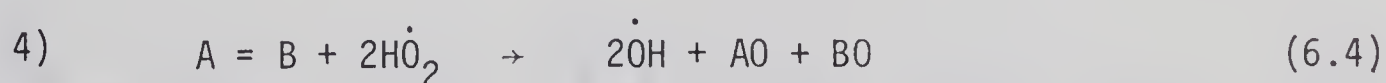
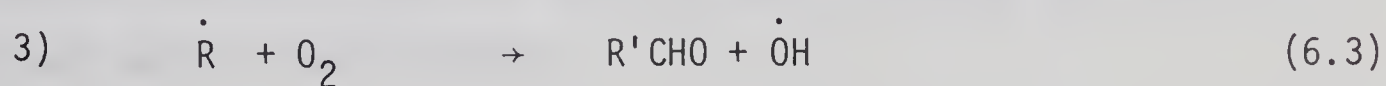
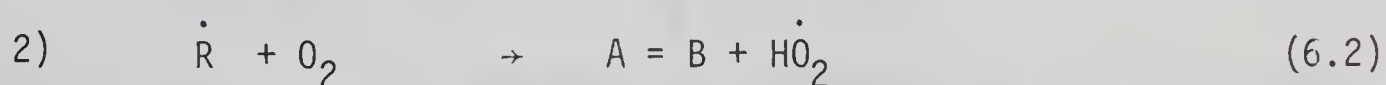
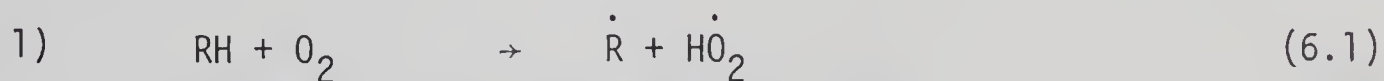
the isomerization scheme and the olefin scheme may be advanced to explain the hydrocarbon oxidation reaction. However, it would not be possible at this stage to make any definitive conclusions in this regard. More experimental data, and especially experimental studies of the elementary steps of the reaction are essential to establish the mechanism of the partial oxidation reaction.

6.6 Reactor Modelling

6.6.1 Simplified Kinetic Models

In absence of a known reaction mechanism and because of the complexity of the hydrocarbon oxidation reaction, attempts have been made to develop a suitable kinetic scheme which can be used for reactor design purposes. Several different mechanisms were postulated, but the following two mechanisms were studied in some detail.

Mechanism I.



RH in the above equations stand for hydrocarbon, A = B for olefins and R'CHO for the aldehydes. The mechanism in essence is a simplified version of a combination of the Semenov scheme and the Knox scheme.

The rate equations for the different species can be obtained by applying the principle of stationary state approximation⁽⁵⁴⁾, a method quite commonly used in chain kinetics. The a's in the equations below for the concentration of the free radicals are rate constants multiplied by the concentration of the molecular species involved.

$$[\text{RC}\dot{\text{O}}] = \frac{a_5}{a_6} \quad (6.10)$$

$$[\dot{\text{R}}] = \frac{2a_1 + a_5}{a_8} \quad (6.11)$$

$$a_7[\dot{\text{O}}\text{H}] = \frac{(a_2 + a_3)(2a_1 + a_5)}{a_8} + a_1 + a_5 \quad (6.12)$$

$$2a_4[\dot{\text{H}}\text{O}_2]^2 = a_1 + a_5 + \frac{a_2}{a_8} (2a_1 + a_5) \quad (6.13)$$

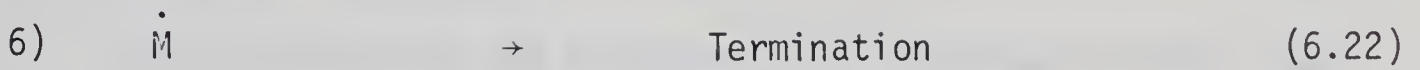
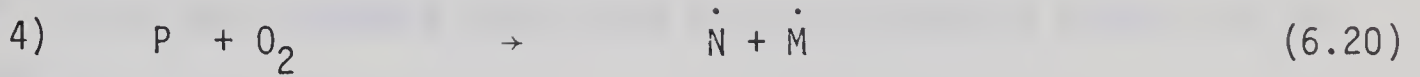
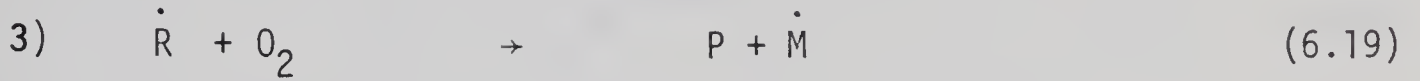
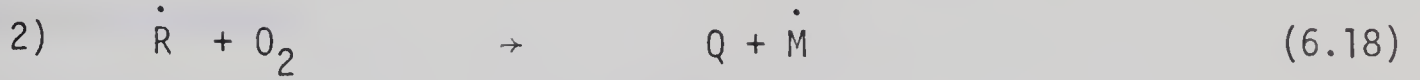
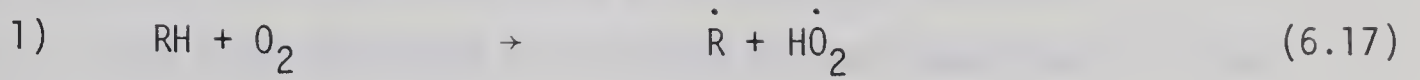
Denoting the concentrations of RH, O₂ and R'CHO by C_A, C_B and C_C, respectively and on simplification,

$$-\frac{dC_A}{dt} = 2K_1C_AC_B + K_5C_BC_C + \frac{K_2+K_3}{K_8} (2K_1C_AC_B + K_5C_BC_C) + K_9C_A \quad (6.14)$$

$$-\frac{dC_B}{dt} = 3K_1C_AC_B + 3K_5C_BC_C + \frac{K_2+K_3}{K_8} (2K_1C_AC_B + K_5C_BC_C) \quad (6.15)$$

$$\frac{dC_C}{dt} = \frac{K_3}{K_8} (2K_1C_AC_B + K_5C_BC_C) - K_5C_BC_C \quad (6.16)$$

Mechanism II



In the above reaction equations, Q and S represent end products, P is an intermediate responsible for branching and $\dot{\text{N}}$ and $\dot{\text{M}}$ are free radical species. On simplification, the rate equations in this case become:

$$-\frac{dC_A}{dt} = K_1 C_A C_B + \frac{K_5}{K_6} C_A (2K_1 C_A C_B + K_4 C_B C_C) + K_7 C_A \quad (6.24)$$

$$-\frac{dC_B}{dt} = 2K_1 C_A C_B + K_4 C_B C_C + \frac{K_5}{K_6} C_A (2K_1 C_A C_B + K_4 C_B C_C) \quad (6.25)$$

$$\frac{dC_C}{dt} = [K_1 C_A C_B + \frac{K_5}{K_6} C_A (2K_1 C_A C_B + K_4 C_B C_C)] / (1 + \frac{K_2}{K_3}) - K_4 C_B C_C \quad (6.26)$$

The reactor temperature profile is given by

$$\frac{dT}{dz} = \frac{1}{mC} \left[-4 \frac{hw}{D_r} (T - T_w) + \sum_{i=1}^n r_i \Delta H_i \right], \quad (6.27)$$

which incorporates the heat of reaction terms. n in the above equation is the number of reaction steps in the mechanism involved.

The rate constants are related to the temperature by the Arrhenius relation:

$$K_i = A_i' e^{-E_i/RT} \quad (6.28)$$

where A_i' is the frequency factor and E_i the activation energy for the reaction.

6.6.2 Estimation of Parameters

The estimation of the parameters in a nonlinear kinetic model poses a severe problem. Several methods have been suggested in literature. Kittrel et al⁽⁵⁵⁾ applied iterative nonlinear least squares regression techniques to obtain parameters for heterogeneous kinetic systems. Donnelly and Quon⁽⁵⁶⁾ employed the method of quasilinearization which reduced the system to a system of linear boundary value equations. Ball and Groenweghe⁽⁵⁷⁾ employed a method proposed by Marquardt⁽⁵⁸⁾ who attempted to combine the best features of Gauss-Newton and the steepest descent methods. The Gauss-Newton method is characterized by quadratic convergence when sufficiently close to the final solution point. The steepest descent method works no matter how far away the solution point is, but becomes very slow as the solution point approaches. The proper combination of these methods would thus appear very desirable and would likely give rapid convergence with a desirable lack of sensitivity to initial values of the parameters.

The parameters of the models in the present case are poorly known and the steepest descent method appeared the likely choice for preliminary estimation. A number of variations of the classical method

have been used by several authors and the one by Rosenbrock⁽⁵⁹⁾ was adopted in the present work. The essence of the method is to vary one parameter at a time and then find out the best direction of advance and continue the iterations. The step size is very simply controlled by observing the change in the quantity to be minimized or maximized. The programming is simple and is aptly described by Rosenbrock⁽⁶⁰⁾.

In the actual programming, the pre-exponential factor was modified as

$$A_i' = 10^{-4} \exp (A_i) \quad , \quad (6.29)$$

and the Arrhenius equation was written in the form

$$K_i = 10^{-4} \exp (A_i' - E_i'/T) \quad , \quad (6.30)$$

where $E_i' = \frac{E_i}{R}$.

The rate equations were expressed in terms of conversion rather than concentration and the dependence on time was changed to dependence on the length of the reactor. The temperature was normalized by dividing by a base temperature. Denoting the moles of hydrocarbon, oxygen and the intermediate as N_A , N_B and N_C , the conversions of the components are defined as follows:

For the hydrocarbon,

$$X_A = \frac{N_{A_0} - N_A}{N_{A_0}} \quad (6.31)$$

where N_{A_0} is the initial moles of the hydrocarbon.

For oxygen

$$X_B = \frac{N_{B_0} - N_B}{N_{B_0}} \quad (6.32)$$

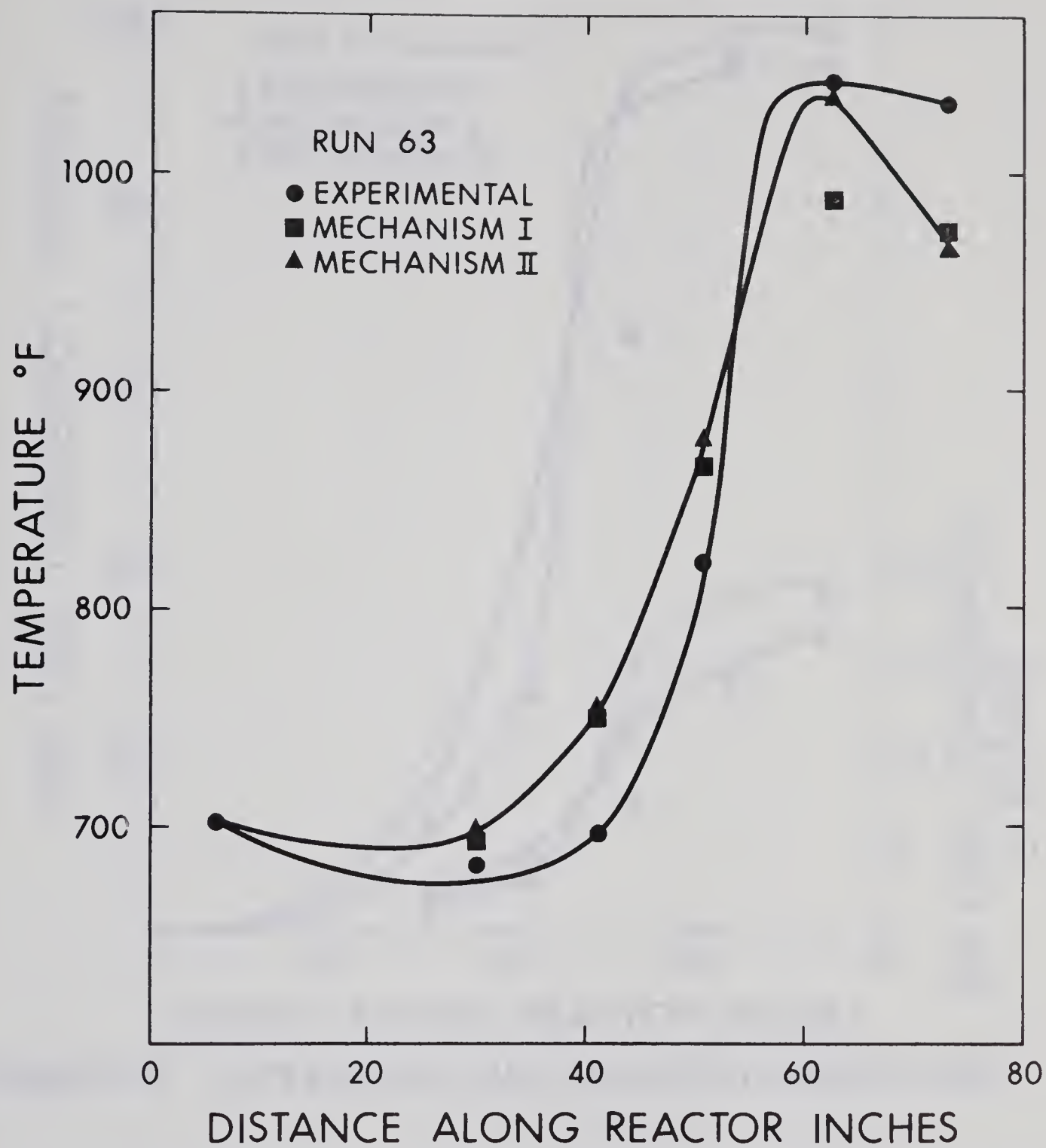


FIGURE 6.24 EXPERIMENTAL AND PREDICTED TEMPERATURE PROFILES

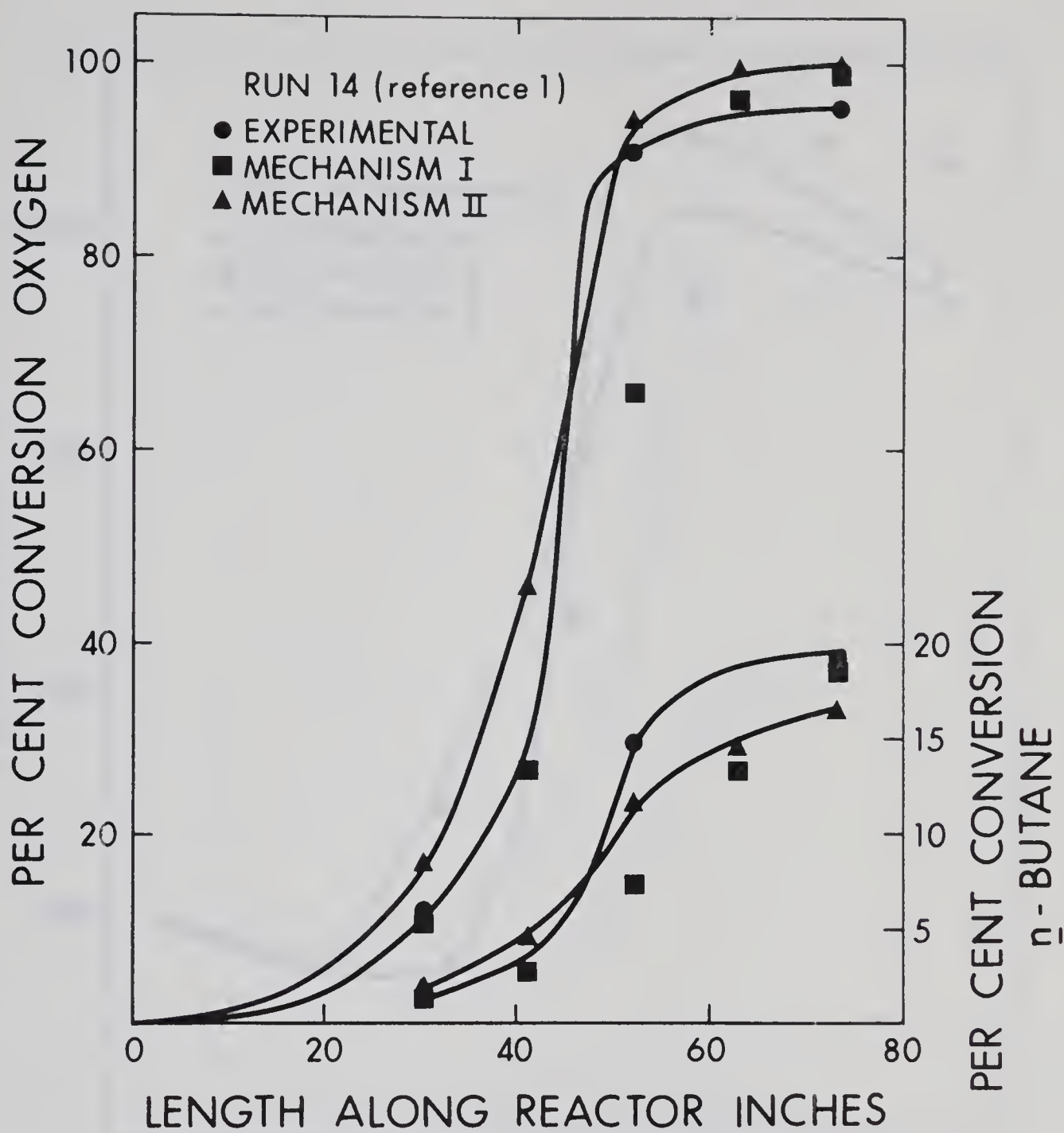


FIGURE 6.25 EXPERIMENTAL AND PREDICTED CONVERSIONS

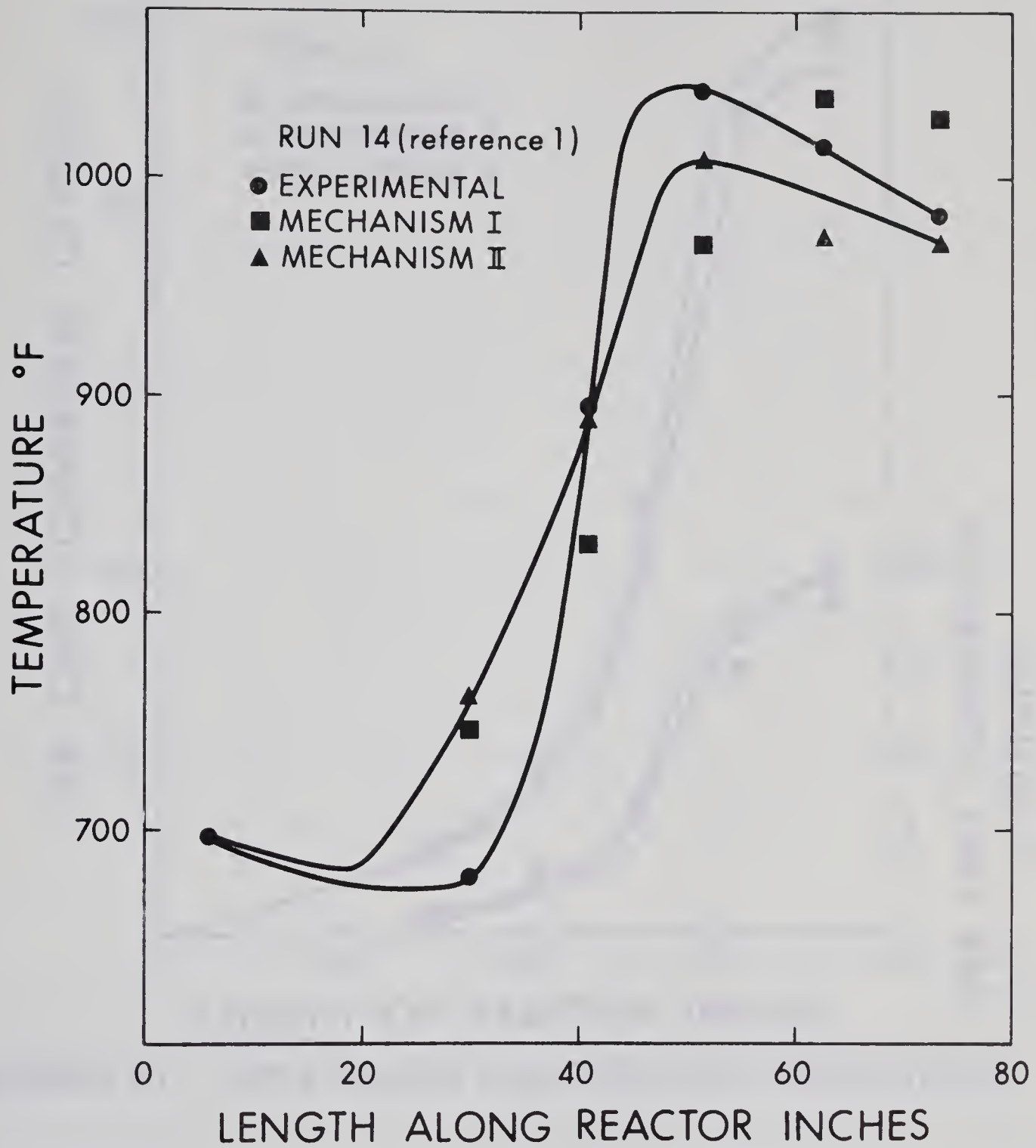


FIGURE 6.26 EXPERIMENTAL AND PREDICTED TEMPERATURE PROFILE

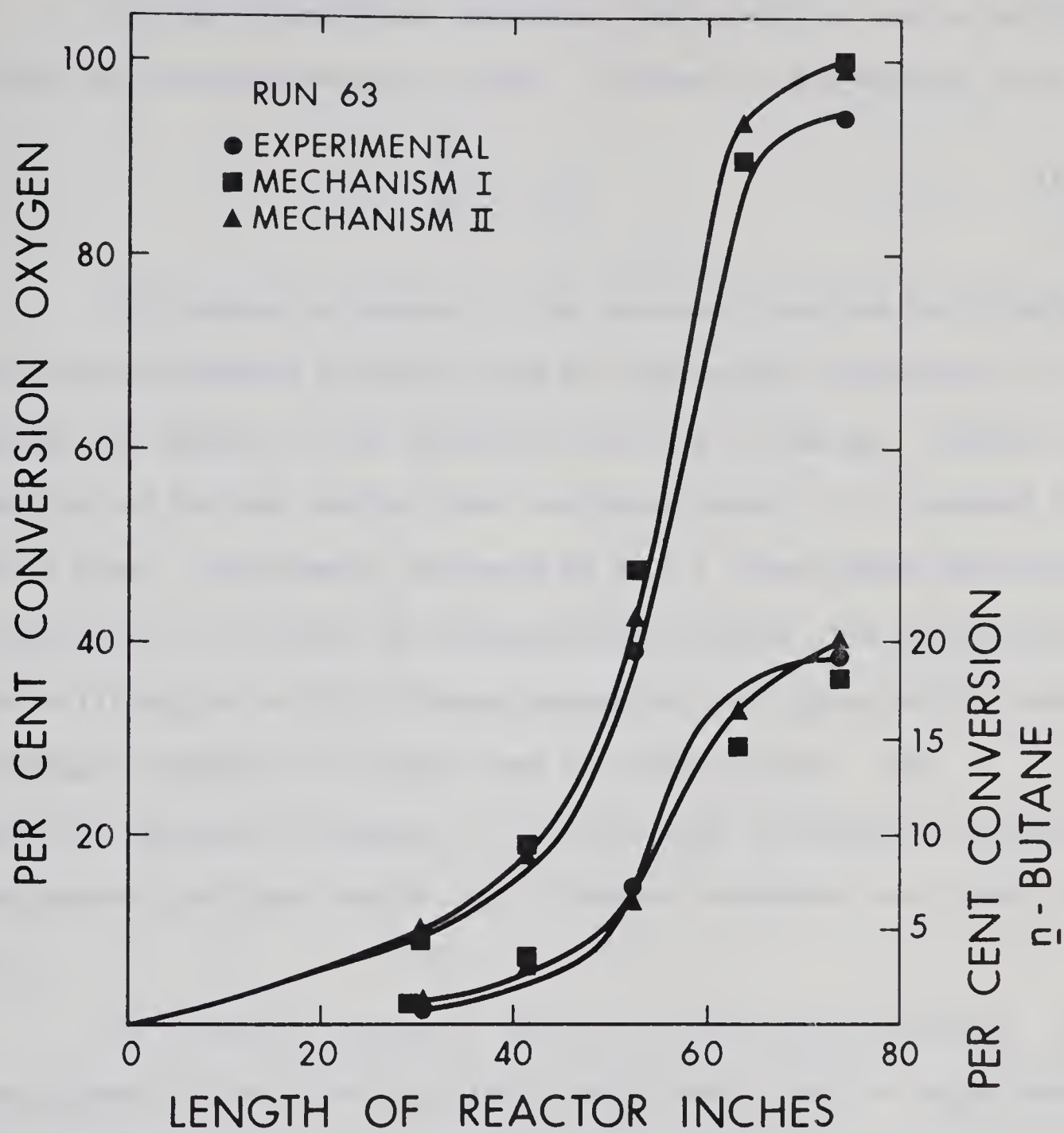


FIGURE 6.27 EXPERIMENTAL AND PREDICTED CONVERSIONS

where N_{B_0} is the initial moles of oxygen.

For the intermediate component, the conversion can be expressed in terms of the hydrocarbon or oxygen. In terms of hydrocarbon, this is

$$X_C = \frac{N_C}{N_{A_0}} \quad (6.33)$$

The unknown parameters in the two models can now be estimated using the experimental data available for the overall conversions of n-butane and oxygen and the temperature profile of the gas. However, on inspection of the two models, there are about twenty or so unknowns in each of them. Simultaneous treatment of such a large number of unknowns is impractical. In order to circumvent this problem, the values available in literature on the different parameters are chosen and the number of unknown parameters is brought down to three or four. Next, a sequential approach is adopted, i.e., the system is solved for three or four unknowns and then another set of unknown parameters are chosen, and so on.

The computer program is general for both the mechanisms. The slope subroutine has to be supplied in each case. Data for experimental runs 60, 62 to 66 and 68 were used in the analysis. Figures 6.24 to 6.27 present the temperature profiles and the conversions as obtained from the models for two runs and compared with the experimental values. Table 6.5 gives the final values of the parameters for the two mechanisms. The parameter values with asterisks were estimated.

TABLE 6.5
Parameter Values of Mechanisms I and II

Reaction Number	Mechanism I			Mechanism II		
	A	E/1000 Btu/lb-mole	$\frac{\Delta H}{1000}$ Btu/lb-mole	A	E/1000 Btu/lb-mole	$\frac{\Delta H}{1000}$ Btu/lb-mole
1	35.0	50.07*	-70.0	34.47*	50.04*	-75.0
2	34.06*	25.0	20.0	$A_2 - A_3$ = 0.0	$E_3 - E_2$ = -5.2*	60.0
3	34.0	27.0	69.8*			70.0
4	-	-	15.0	34.07*	30.44*	-60.0
5	35.0	30.98*	-60.0	$A_5 - A_6$ = 10.0	$E_6 - E_5$ = -9.6*	40.9*
6	-	-	50.0			-15.5*
7	-	-	33.5*	34.68*	53.17*	-40.0
8	34.0	40.0	40.0			
9	35.0	54.02*	0.0			

Table 6.6 gives the variance covariance matrix for three parameters in mechanism II. The parameters considered were the activation energies for the initiation step, the branching step and the overall cracking step -- reactions 1, 4 and 7, respectively. Data for runs 62 to 66 were used to calculate this matrix.

TABLE 6.6

Parameter Estimates: $E_1 = 50.04$ $E_4 = 30.44$ $E_7 = 53.17$

Variance Covariance Matrix

$$\underline{C} = \begin{bmatrix} 1.4142 & -.6966 & -.2857 \\ -.6966 & .3459 & .1384 \\ -.2857 & .1384 & 1.9675 \end{bmatrix}$$

TABLE 6.7

Variance and Standard Deviation

Runs	Mechanism	Variance			Standard Deviation		
		n-butane conversion	oxygen conversion	Temperature $T^* = \frac{T}{1185}$	n-butane conversion	oxygen conversion	Temperature T
Homogeneous Runs	I	5.68×10^{-4}	1.59×10^{-2}	2.71×10^{-3}	0.024	0.126	61.5
	II	4.86×10^{-4}	1.21×10^{-2}	2.01×10^{-3}	0.022	0.110	53.0
Transported Bed Runs*	I	1.0×10^{-3}	3.78×10^{-2}	2.93×10^{-3}	0.0316	0.194	63.7
	II	5.45×10^{-4}	2.34×10^{-2}	9.36×10^{-4}	0.0233	0.152	36.2
Independent Runs**	I	1.40×10^{-3}	4.47×10^{-2}	3.20×10^{-3}	0.0384	0.211	66.8
	II	2.73×10^{-4}	1.31×10^{-2}	3.61×10^{-3}	0.0165	0.114	71.5

* To be dealt with in section 7.4.

** Reference 1.

The two models were also used to predict the temperature profiles and conversions for a number of runs made by Anderson⁽¹⁾ earlier in this laboratory. The runs used from his results were runs 11, 12, 13, 14 and 17. Table 6.7 shows the variance and standard deviation for the present runs and the runs by Anderson for n-butane conversion, oxygen conversion and temperature profile. It is seen that for the present runs, there is a slight edge of mechanism II compared to mechanism I. For the other set of runs, mechanism II is considerably better than mechanism I. The two sets of data above cover a range of starting temperatures from 680°F to 708°F and starting n-butane to oxygen ratios of 14.0 to 7.0. The predictions by the two models in this fairly large range of operating conditions have been quite good. This, however, does not mean that either mechanism is taking place in the reactor. The establishment of a mechanism of the reaction is a much larger problem and the present models are used only to predict the overall conversions and temperature profiles in the reactor under the operating conditions as stated.

6.7 Summary

The temperature profiles and overall conversions of n-butane and oxygen are consistent and agree with other results in this area. The product distribution data suggest that a combination of the aldehydic scheme of Semenov and Shtern and the olefinic scheme of Knox may be taking place in the reactor. However, the interpretation of all the data were difficult and were associated with considerable uncertainty because of the high sensitivity of the ordinate with a relatively small change in the abscissa in most of the cases.

An attempt has been made to develop a suitable kinetic scheme

for the reaction. This attempt has been limited to the prediction of temperature profiles and overall conversions for the different runs. Two schemes have been given particular attention and their parameters obtained by a numerical method. The schemes have been tested against independent experiments in an earlier work and the two models, especially model II predict the temperature profiles and overall conversions quite well. The variance and standard deviation in each case are presented.

CHAPTER VII

TRANSPORTED BED REACTOR: RESULTS AND DISCUSSIONS

7.1 Introduction

A mathematical model for a transported bed reactor has been formulated and a numerical method developed to solve the problem. Effects of particle size and loading ratio on the gas and solid temperature profiles are investigated.

The performance of the transported bed reactor in the partial oxidation of n-butane with air is evaluated. The selectivity of different products are compared with those obtained in a homogeneous reactor. The effect of additional surface in a transported bed reactor is evaluated.

The kinetic models for the homogeneous reactor are used to predict the temperature profiles and conversions in the transported bed reactor.

7.2 Evaluation of Heat Transfer Characteristics

A preliminary study of the behaviour of a transported bed system was required to evaluate its heat transfer characteristics. This was done with particular emphasis on the effect of a radial variation in particle temperatures. In earlier studies on heat transfer in transport lines, the solids temperature has been considered uniform across the cross section⁽⁶¹⁾. While it would be true for very small particles, the larger particles may have temperature variations large enough to affect the results.

Basic equations for momentum and heat transport for a gas solids system were developed by Soo et al^(62,63). Efforts to take into

account the velocity profiles of the solid particles and their concentration distributions were not conclusive⁽⁶⁴⁾ and it was assumed that these could be taken care of by lumped parameters. Experimental investigations of the heat transfer characteristics of a two phase system were made by Farbar and Depew⁽⁶⁵⁾ and Abel and coworkers⁽⁶⁶⁾. A general increase in the gas to wall heat transfer was reported for a gas-solids system. The particle diameter and the solids to gas loading ratios were the two main variables, but a satisfactory correlation was not available for a wide range. Studies of the drag coefficients for a particulate system has been made by several investigators; the results are not definitive, but suggest that standard drag coefficients for single spheres can be used for the transport system⁽⁶⁷⁾.

Practically no work has been reported in literature on the gas to solids heat transfer coefficients, mainly because of the experimental difficulties involved in such studies. In most heat transfer studies in gas solids systems, the temperature difference between the gas and solids was small and reliable measurement of this difference was not possible. Chukhanov⁽⁶⁸⁾ made an attempt to use the data for fixed spheres in a moving gas. The gas to solids heat transfer coefficient in this study was obtained from Gröber⁽⁶⁹⁾ and the gas to wall heat transfer coefficient was obtained from Farbar and Morley⁽⁷⁰⁾.

The following equations can be derived for the reactor system:

Continuity equations -- consideration of continuity for the gas phase only gives for a perfect gas

$$\frac{m}{A_r} = \frac{u}{v} = \frac{uP}{RT} \quad (7.1)$$

The concentration of the solid particles is given by

$$m_p = m_p^* \frac{u}{u_p}, \quad (7.2)$$

which accounts for the fact that higher velocity of the solid particles shows up as a decrease in concentration of the solids.

Overall energy equation -- consideration of heat transfer to the wall and the generation of heat because of the reaction leads to the equation, for one pound of gas;

$$d[CT + m_p C_p T_p] = - \frac{h_w A_w}{m} (T - T_w) dZ + \frac{\epsilon A_r}{m} \sum_{i=1}^n r_i (-\Delta H_i) dZ, \quad (7.3)$$

which can be put in the form

$$\frac{dT}{dZ} = \frac{1}{mC} \left[-4 \frac{h_w}{D_r} (T - T_w) - h_c A_s (T - v_s) + \epsilon \sum_{i=1}^n r_i (-\Delta H_i) \right], \quad (7.3)$$

where n is the number of rate equations.

Solids energy balance -- heat is received by the solids from the gas by convection:

$$d[m_p C_p T_p] = \frac{h_c A_s}{m} (T - v_s) dZ$$

$$\frac{dT_p}{dZ} = \frac{h_c A_s}{m_p C_p m} (T - v_s) \quad (7.4)$$

Momentum of solid particles -- the solids are conveyed by the viscous drag exerted by the gaseous stream. The rate of change of momentum can be expressed as

$$g_c - F(u - u_p) = u_p \frac{d u_p}{dZ} \quad (7.5)$$

where the time lag of fluid-solid motion (sec^{-1}) $F = \frac{3}{4} \frac{C_D}{d_p} \frac{\rho}{\rho_p} |u - u_p|$, and the drag coefficient are functions of the particle Reynolds number

$$Re_p = \frac{d_p |u - u_p| \rho}{\mu}$$

Overall momentum equation -- since the solid particles are driven by the gas, the momentum balance gives

$$\frac{dP}{\rho} + \frac{u du}{g_c} + \frac{m_p u_p du_p}{g_c} + \frac{2u^2 f}{g_c D_r} dZ + dZ \frac{\rho_p s}{\rho} = 0$$

Combining with the continuity equation and solids momentum equations leads to

$$\frac{du}{dZ} \left(\frac{1}{u} - \frac{u}{g_c RT} \right) = \frac{1}{T} \frac{dT}{dZ} + \frac{m_p u_p}{g_c RT} \frac{du_p}{dZ} + \frac{2u^2 f}{g_c RT D_r} + \frac{1}{g_c RT} \frac{\rho_p s}{\rho} \quad (7.6)$$

Gas phase material balance -- material balance for a small increment of length dZ gives

$$\frac{dx_i}{dZ} = \frac{\epsilon}{G_o y_o} r_i, \text{ where} \quad (7.7)$$

$r_i = \xi(\underline{x}, \underline{K}, T)$, and is derived in appendix F. ϵ is the void fraction and is defined as

$$\begin{aligned} \epsilon &= 1 - \frac{\text{volume of solids}}{\text{total volume}} \\ &\approx 1 - \frac{\text{volume of solids}}{\text{volume of gas}} \\ &= 1 - \frac{w_p / \rho_p}{m / \rho} \\ &= 1 - m_p \frac{\rho}{\rho_p} \end{aligned} \quad (7.8)$$

A_s is the solids surface area per ft reactor and is given by

$$A_s = \pi d_p^2 \times N, \text{ where } N = \text{no. of particles per ft reactor.}$$

$$\begin{aligned}
 N &= w_p \frac{\text{lb solid}}{\text{hr}} \frac{1}{u_p} \frac{\text{hr}}{\text{ft}} \frac{1}{\rho_p} \frac{\text{ft}^3}{\text{lb solid}} \frac{1}{1/6 \pi d_p^3} \frac{1}{\text{ft}^3} \\
 &= \frac{6 w_p}{u_p \rho_p d_p}
 \end{aligned} \tag{7.9}$$

Combining equation (7.4) with the above gives,

$$\frac{dT_p}{dZ} = \frac{6 h_c}{u_p \rho_p d_p C_p} (T - v_s) \tag{7.10}$$

Heat conduction equation into the solids -- the radial temperature distribution of the solid particles is given by

$$\frac{\partial v}{\partial t} = \frac{\alpha}{r_p^2} \frac{\partial}{\partial r_p} (r_p^2 \frac{\partial v}{\partial r_p}) \tag{7.11}$$

The time and length of the reactor are simply related by

$$\frac{dZ}{dt} = u_p \tag{7.12}$$

The boundary condition for the partial differential equation is given by a heat balance at the gas solids interface.

$$\left. \frac{\partial v}{\partial r_p} \right|_{r_p=R_p} = \frac{h_c}{K_s} (T - v_s) \tag{7.13}$$

The initial condition is

$$v(0, r_p) = \phi(r_p) \tag{7.14}$$

By symmetry,

$$\left. \frac{\partial v}{\partial r_p} \right|_{r_p=0} = 0 \tag{7.15}$$

The system thus consists of a set of nonlinear first order ordinary differential equations and a second order parabolic partial differential equation. The solution is difficult because of the coupling boundary condition (7.13) for the partial differential equation. The method of solution found successful decouples the two sets by replacing the coupling boundary condition for the solids surface temperature by an explicit function of time. The gas and solids equations are now solved separately and the energy changes in both phases calculated. The function is adjusted until the overall energy balance checks.

It is assumed that for a small increment of time, the solids surface temperature changes linearly, e.g.,

$$v_s = v_s^{(0)} + b \tau$$

where the superscript "0" signifies the beginning of the time increment and b is some constant to be determined by matching the enthalpy changes in the gas and solid phases.

A semianalytical technique is used to obtain a solution of the partial differential equation⁽⁷¹⁾. In this method, the space derivatives are discretised and a set of difference differential equations are obtained. The derivation of the partial differential equation and the discretisation are shown in Appendix F. The discretised equation can be written in the form

$$\underline{G} \frac{d\underline{y}}{d\theta} = \underline{B} \underline{y} + \underline{S}(\theta) \quad (7.16)$$

Certain properties of matrix algebra are now used to obtain a solution of the matrix differential equation in a closed form as

$$\underline{y}(\theta, r_p) = \underline{G}^{-1/2} \underline{Q} \underline{E}(\theta) \underline{Q}^T \underline{G}^{1/2} [\underline{y}^{(0)} + \int_0^\theta \underline{G}^{-1/2} \underline{Q} \underline{E}^{-1}(\sigma) \underline{Q}^T \underline{G}^{-1/2} \underline{S}(\sigma) d\sigma] \quad (7.17)$$

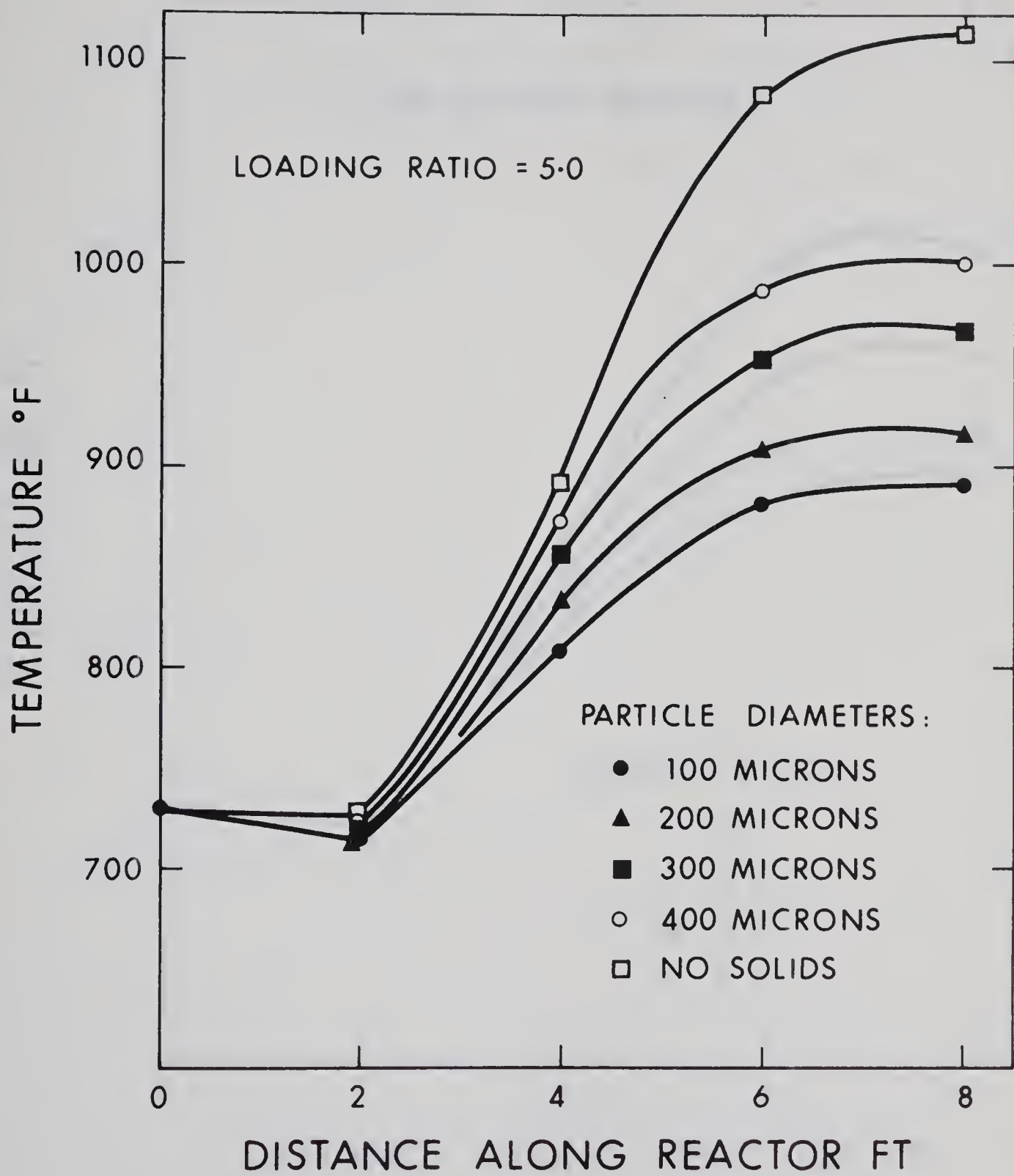


FIGURE 7.1 GAS TEMPERATURE-EFFECT OF PARTICLE SIZE

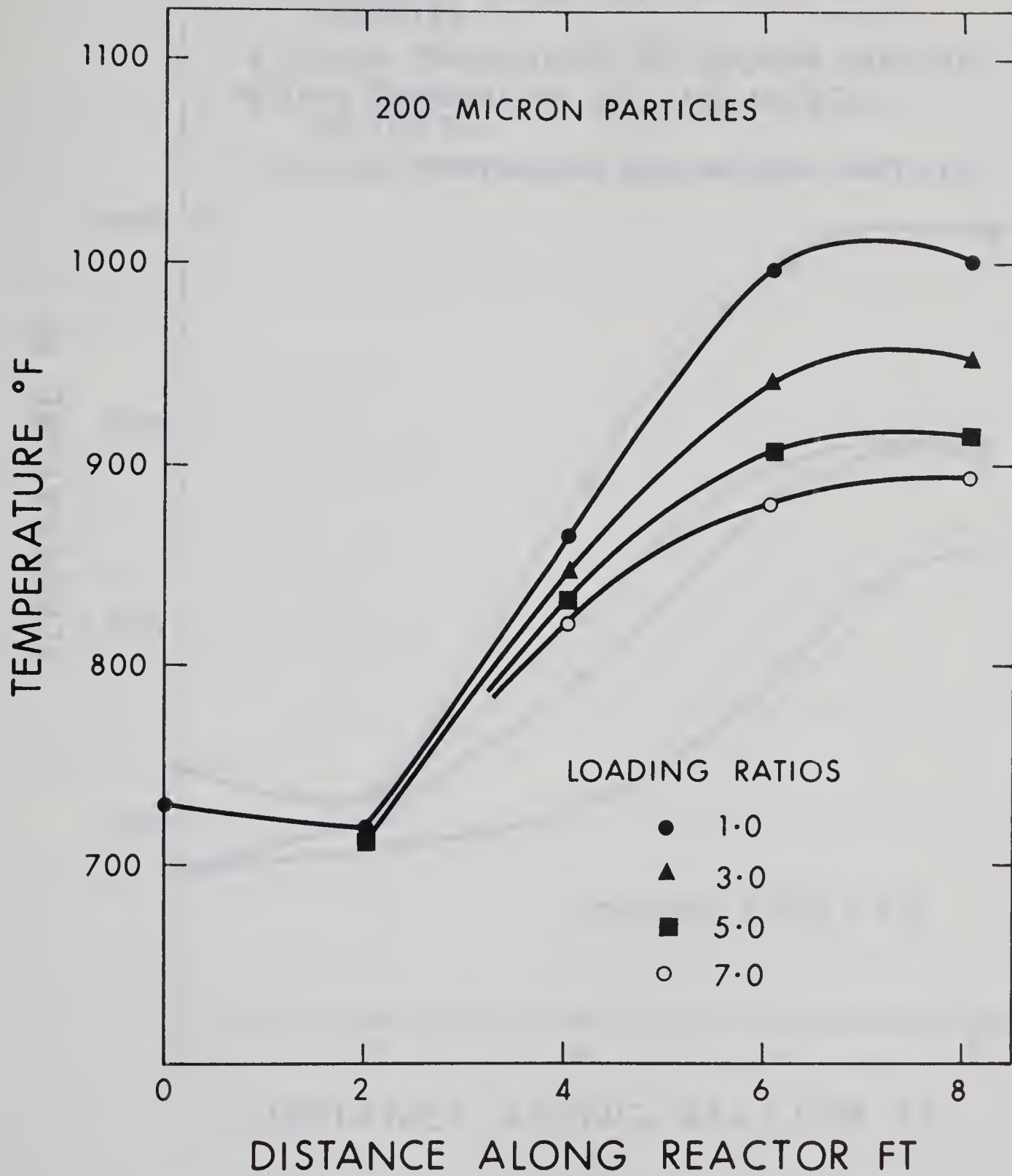


FIGURE 7.2 GAS TEMPERATURE-EFFECT OF LOADING RATIO

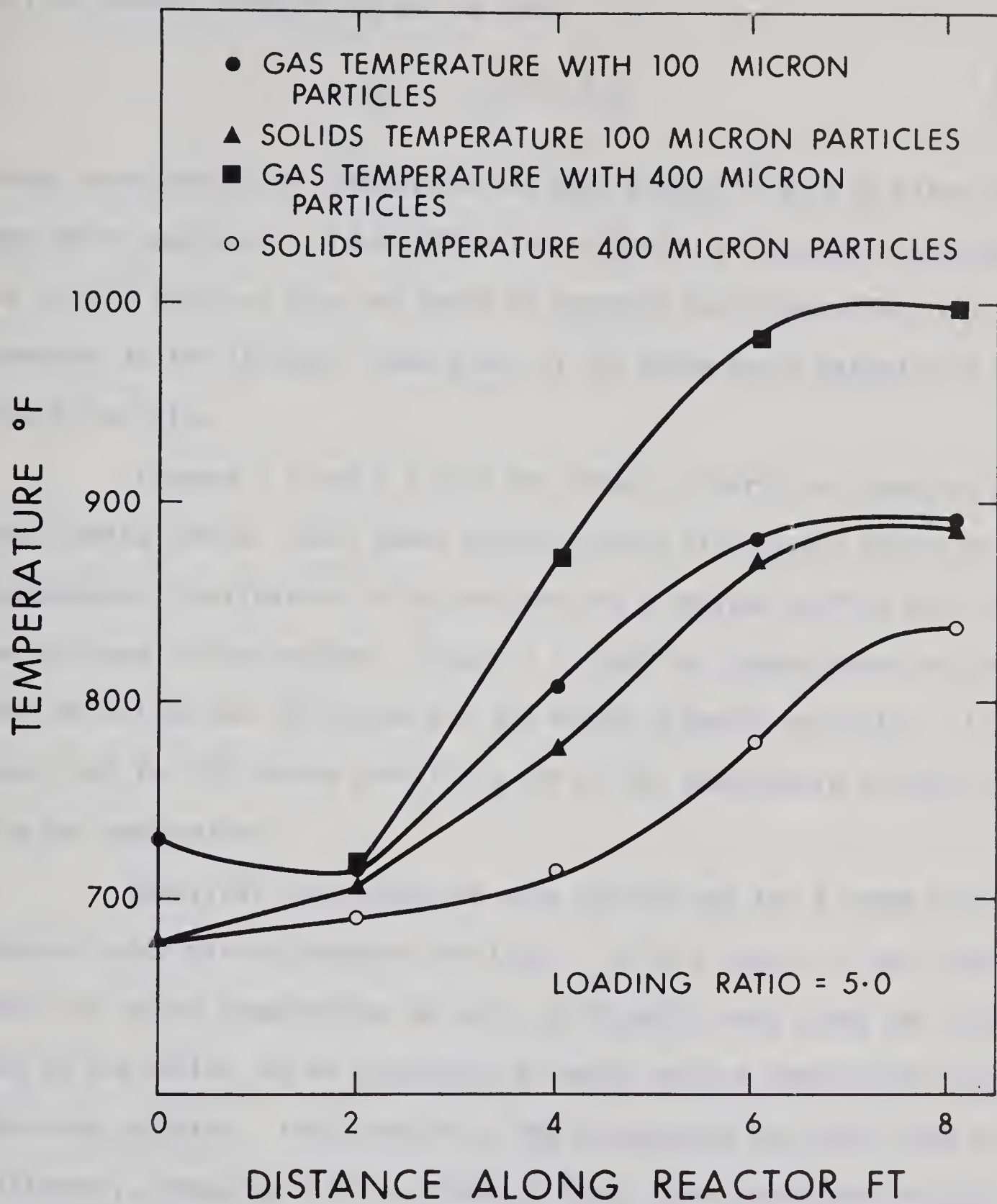


FIGURE 7.3 TEMPERATURES OF GAS AND SOLIDS PHASES

To solve the gas phase equations, a time average value of the solids surface temperature can be used.

$$v_s = v_s^{(0)} + \frac{b \tau}{2}$$

Runge Kutta method of integration has been generally used to solve the gas phase equations. The modification of Merson discussed by Lapidus⁽⁷²⁾ to control the step size was found to decrease the integration time, as compared to the straight forward use of the Runge Kutta method with a fixed step size.

Figures 7.1 and 7.2 show the effect of particle diameters and the loading ratios. Both these variables have significant effect on the temperature distribution in the reactor and a desired profile can likely be achieved in the reactor. Figure 7.3 shows the temperatures of the gas and solids for 100 micron and 400 micron diameter particles. It is seen that for 100 micron particles, the solids temperature follows closely the gas temperature.

Numerical investigations were carried out for a range of 50 micron to 800 micron diameter particles. In this range, it was found that the solids temperatures do not significantly vary along the radius and so the solids can be considered to reach uniform temperature across the cross section. This simplifies the transported bed model very significantly, reducing it to a system of first order nonlinear ordinary differential equations. This in turn makes the parameter estimation problem of a transported bed reactor much easier.

In cases where a larger range of particle diameters are used, the numerical method presented in this section can be readily used to solve the problem and to check the validity of the simplification offered

by the use of uniform particle temperature.

7.3 Experimental Investigations

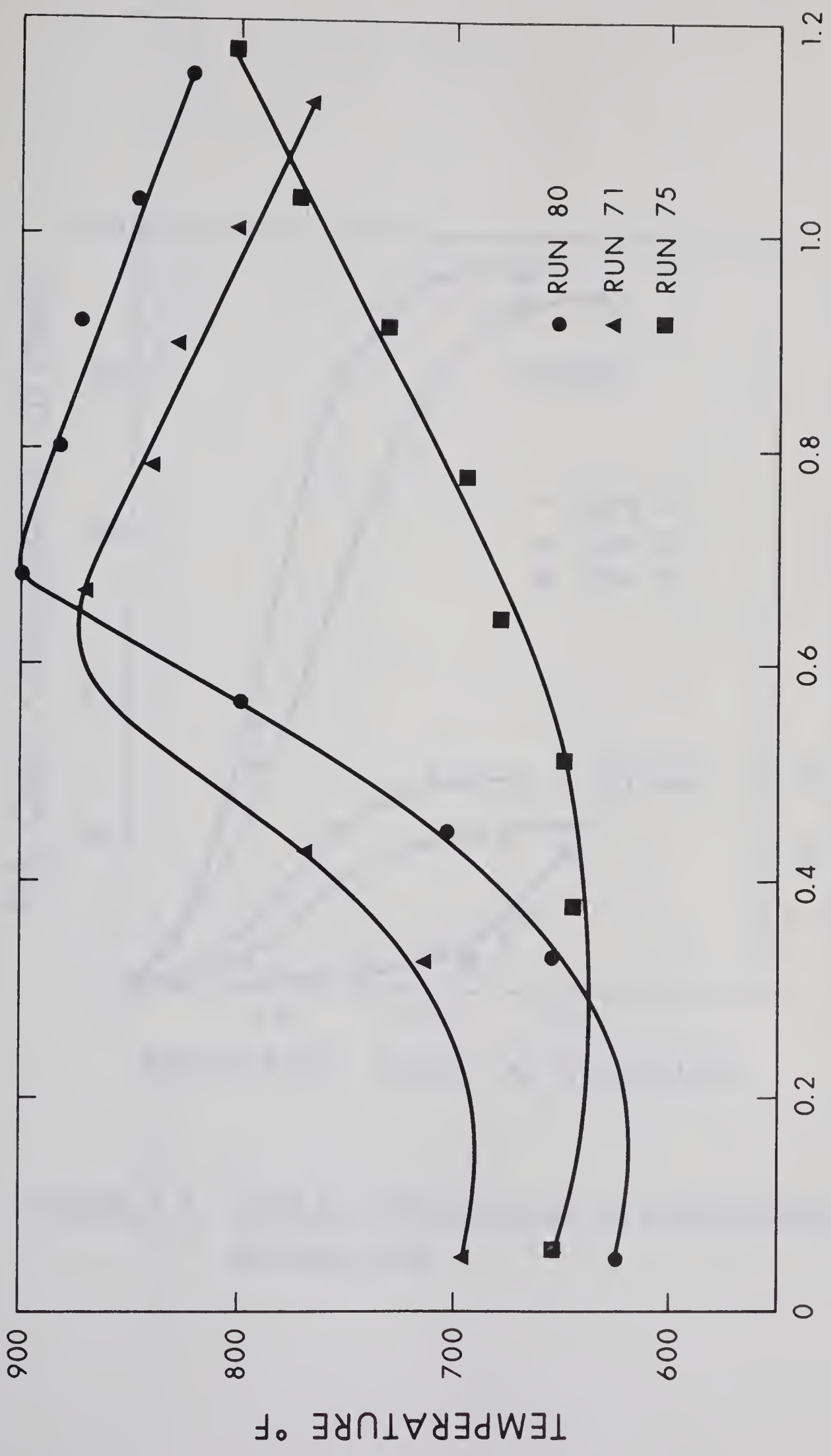
7.3.1 Results from Transported Bed Reactor

A number of runs were conducted in the transported bed reactor in order to obtain the temperature profiles, overall conversions and the product selectivity, and to compare with those of the homogeneous reactor. The experimental runs are summarized in Table 7.1 and the temperature profiles are presented in Table D.2 in the appendix.

The solids flow rates were measured by weighing the total amount of solids collected for each run. The capacity of the feeder was limited by the dimension of the rectangular slots cut into the rotor in the solids feeder. The feeder becomes unstable if operated beyond 70-80 rpm. The reactor, therefore, could not be operated at loading ratios higher than 3.0 to 5.0. For such loading ratios, the maximum temperature of the reactor was reduced by about 150°F. The temperature profile was flattened and so also the conversions. Figures 7.4 and 7.5 show the temperature profiles and conversions for some of the runs.

7.3.2 Comparison with Homogeneous Reactor

Figures 7.6 to 7.11 show the comparison for two runs, run 65 for the homogeneous reactor and run 77 for the transported bed reactor, both conducted at the same hydrocarbon to oxygen ratio. There is a difference of 140°F in the maximum temperature obtained, and the final yield of the oxygenated products increases from 0.30 mole/mole n-butane reacted for the homogeneous run to 0.50 mole/mole n-butane reacted for the TBR. Much of this increase results from an increased amount of methanol whose amount rises from 0.17 mole/mole n-butane reacted to 0.30 mole on the same basis. There is some increase in the amount of the olefins and a



RESIDENCE TIME IN SECONDS

FIGURE 7.4 GAS TEMPERATURE PROFILES IN TRANSPORTED BED REACTOR

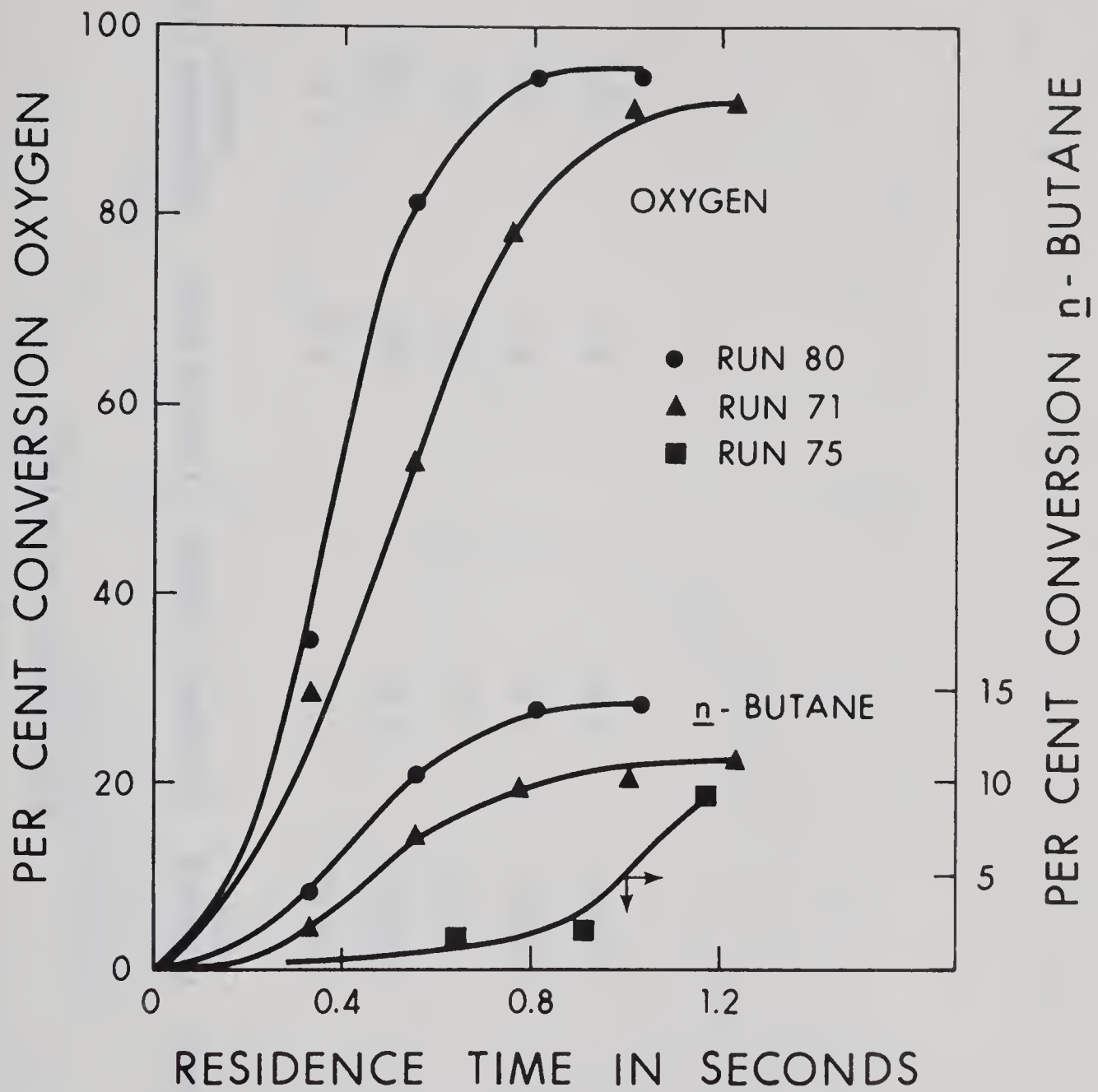


FIGURE 7.5 OVERALL CONVERSIONS IN TRANSPORTED BED REACTOR

TABLE 7.1

EXPERIMENTAL RUN DETAILS

Run Number	Inlet Temperature °F	Pressure psia	n-butane: oxygen	Loading Ratio	Residence Time second	Inlet Reynolds Number
71	698	51.40	10.7	3.0	1.25	6402
73	678	53.72	9.4	3.0	1.38	6015
75	655	51.35	8.4	5.0	1.44	5492
77	650	53.50	7.4	4.0	1.27	6245
80	625	53.50	6.8	3.2	1.26	6412

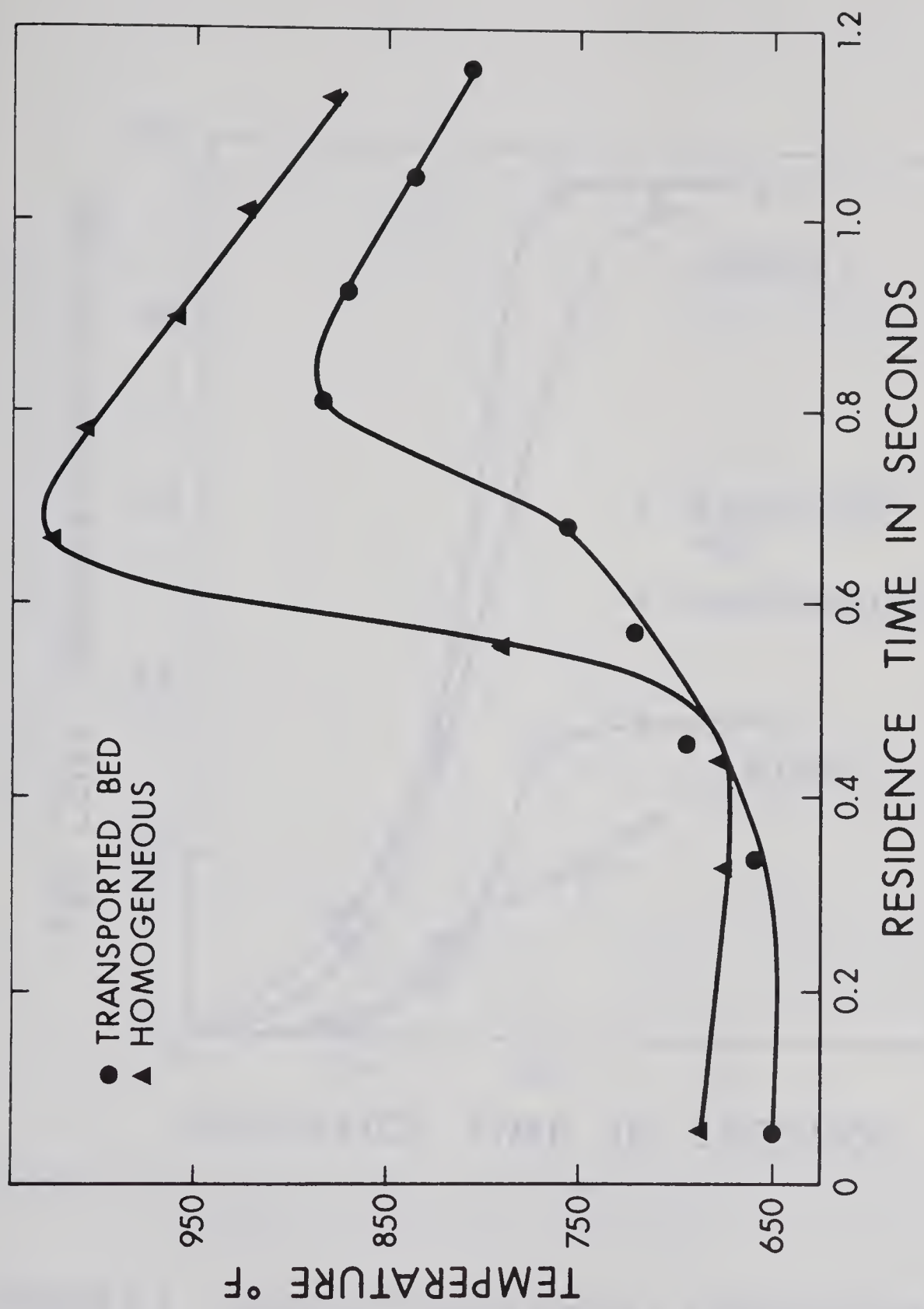


FIGURE 7.6 TEMPERATURE PROFILES: COMPARISON BETWEEN HOMOGENEOUS AND TRANSPORTED BED RUNS

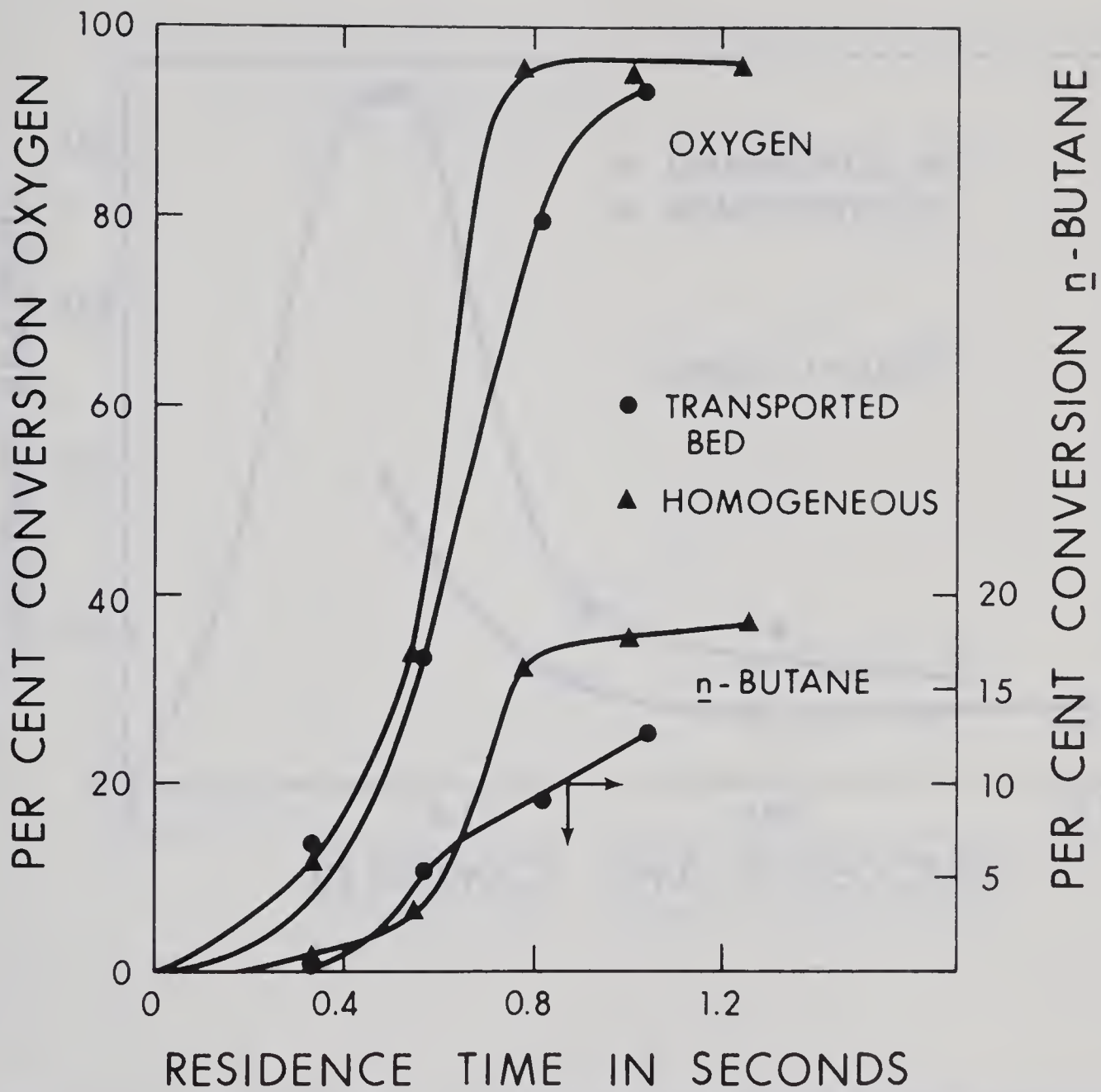


FIGURE 7.7 OVERALL CONVERSIONS - COMPARISON BETWEEN HOMOGENEOUS AND TRANSPORTED BED RUNS

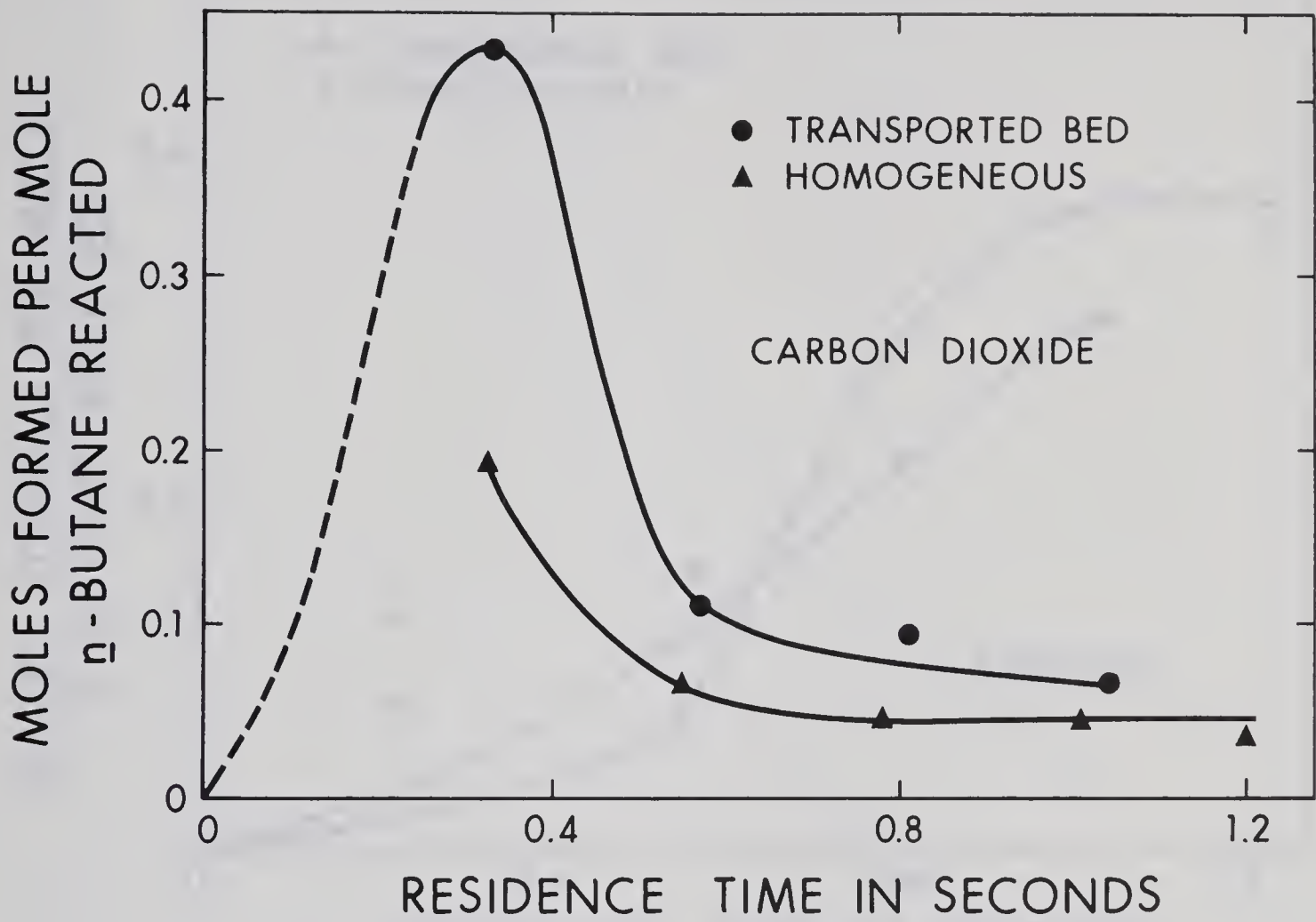


FIGURE 7.8 SELECTIVITY - COMPARISON BETWEEN HOMOGENEOUS AND TRANSPORTED BED RUNS

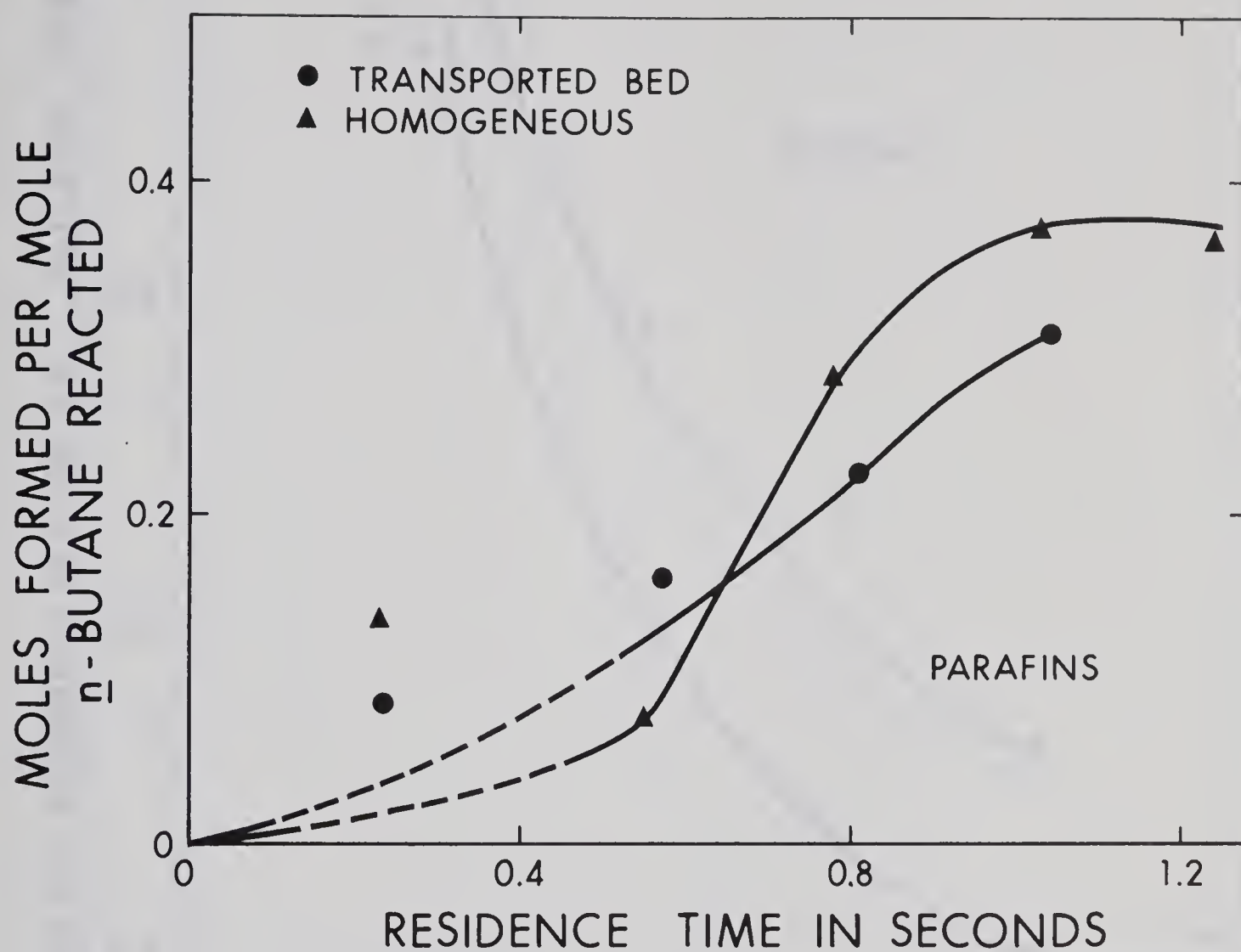


FIGURE 7.9 SELECTIVITY - COMPARISON BETWEEN HOMOGENEOUS AND TRANSPORTED BED RUNS

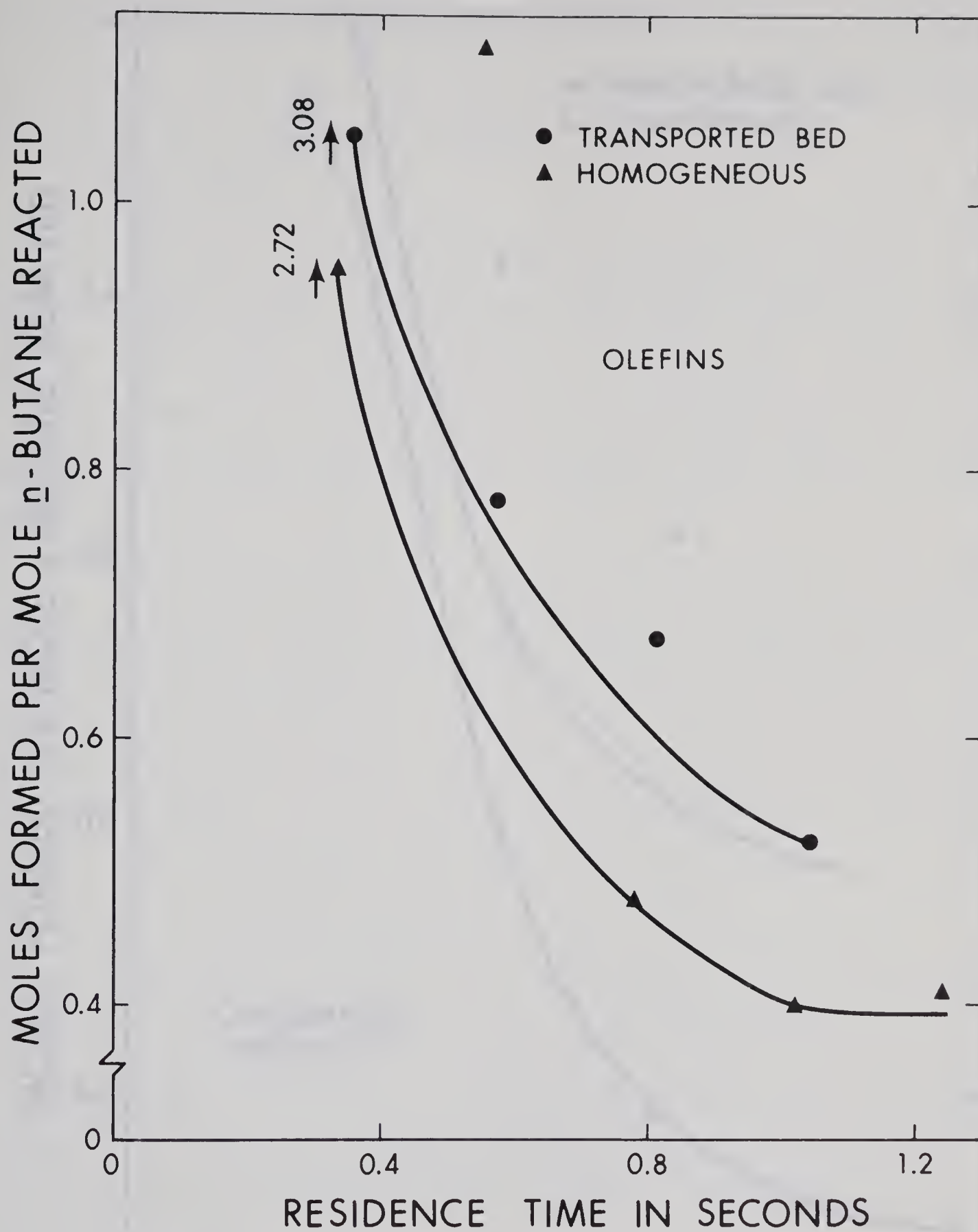


FIGURE 7.10 SELECTIVITY - COMPARISON BETWEEN HOMOGENEOUS AND TRANSPORTED BED RUNS

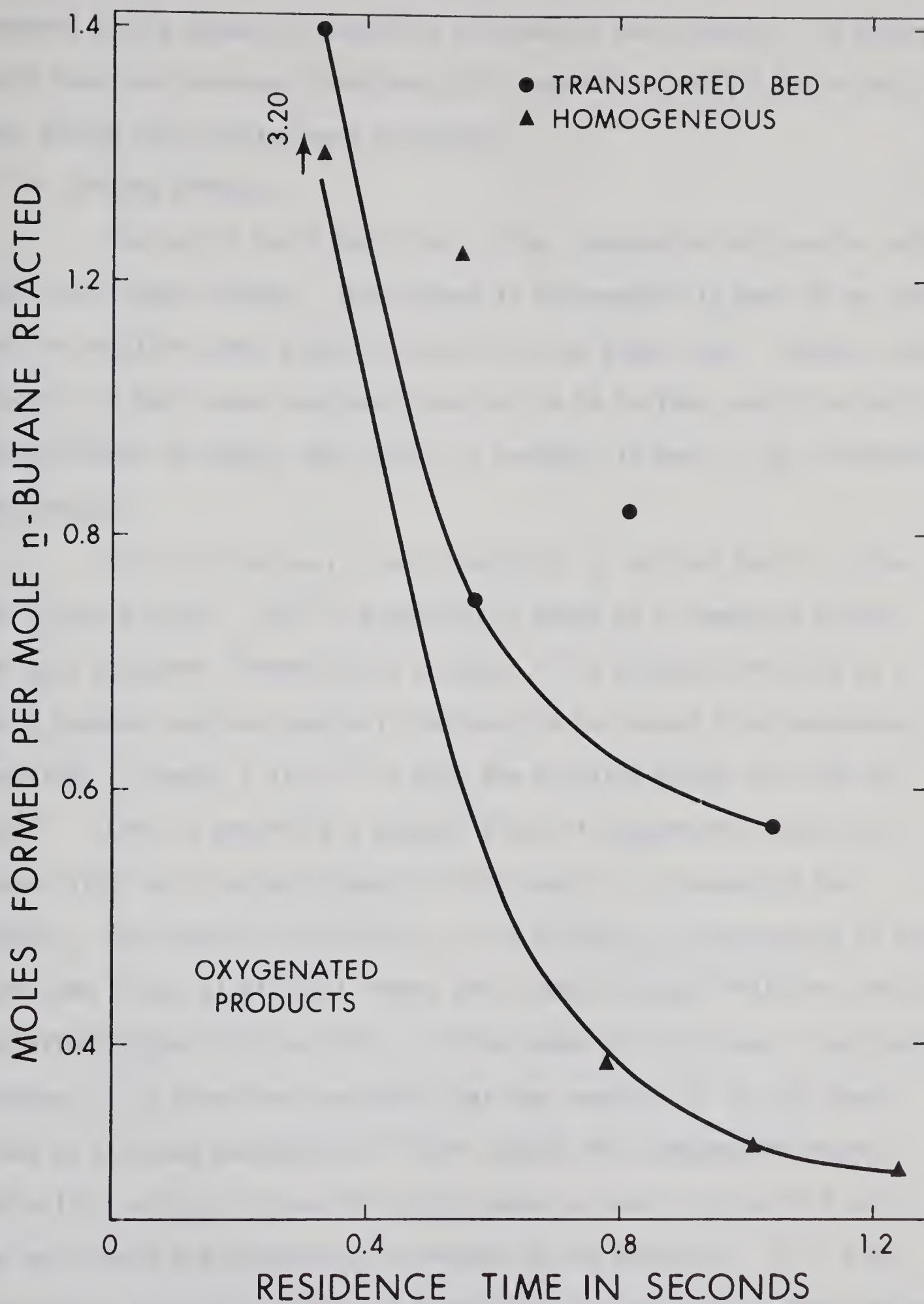


FIGURE 7.11 SELECTIVITY - COMPARISON BETWEEN HOMOGENEOUS AND TRANSPORTED BED RUNS

decrease in the amount of paraffins obtained in the reactor. The time of rapid reaction increases from about 0.15 seconds to about 0.25 seconds, thus making the reaction more tractable.

7.3.3 Surface Effects

The use of solid particles in the transported bed reactor introduces additional surface. The voidage in the reactor is over 99 per cent and the reaction takes place essentially in an empty tube. However, the reaction in many cases have been reported to be surface sensitive and it was desirable to obtain the effects of surface, if any, in the transported bed reactor.

For this purpose, a new selectivity is defined and is called the relative yield. This is expressed as moles of a component formed per mole n-butenes formed in the reaction. The butenes were used as a basis because they are generally believed to be formed from homogeneous reactions. Figures 7.12 to 7.16 show the relative yields for runs 65 and 77. There is generally a greater yield of oxygenated products and lesser yield of cracking products in the case of a transported bed reactor. The product distribution is not altered in the presence of solid particles to any significant extent which would suggest that the surface has affected the relative yield. In the range of the present experimental program, it is therefore concluded that the reaction in the TBR took place by the same mechanism as in the case of the homogeneous reactor. The solid particles in the TBR simply acted as heat sink and did not in any way change the homogeneous character of the reaction. It is also argued that since the additional surface did not reveal any effect of the surface, the formation of all the products in the partial oxidation of n-butane takes place homogeneously. The present study therefore did not

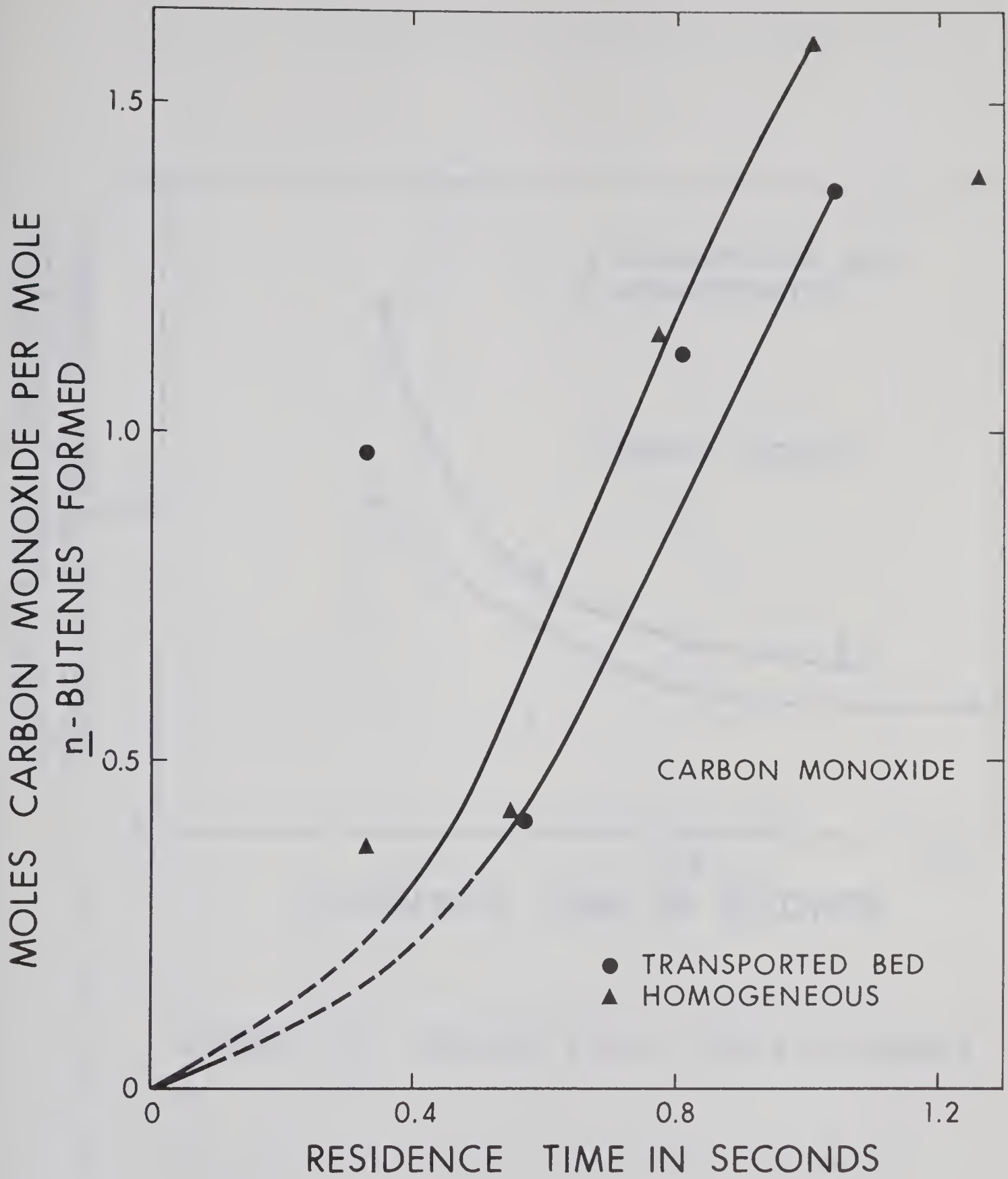


FIGURE 7.12 RELATIVE YIELD - EFFECT OF SURFACE

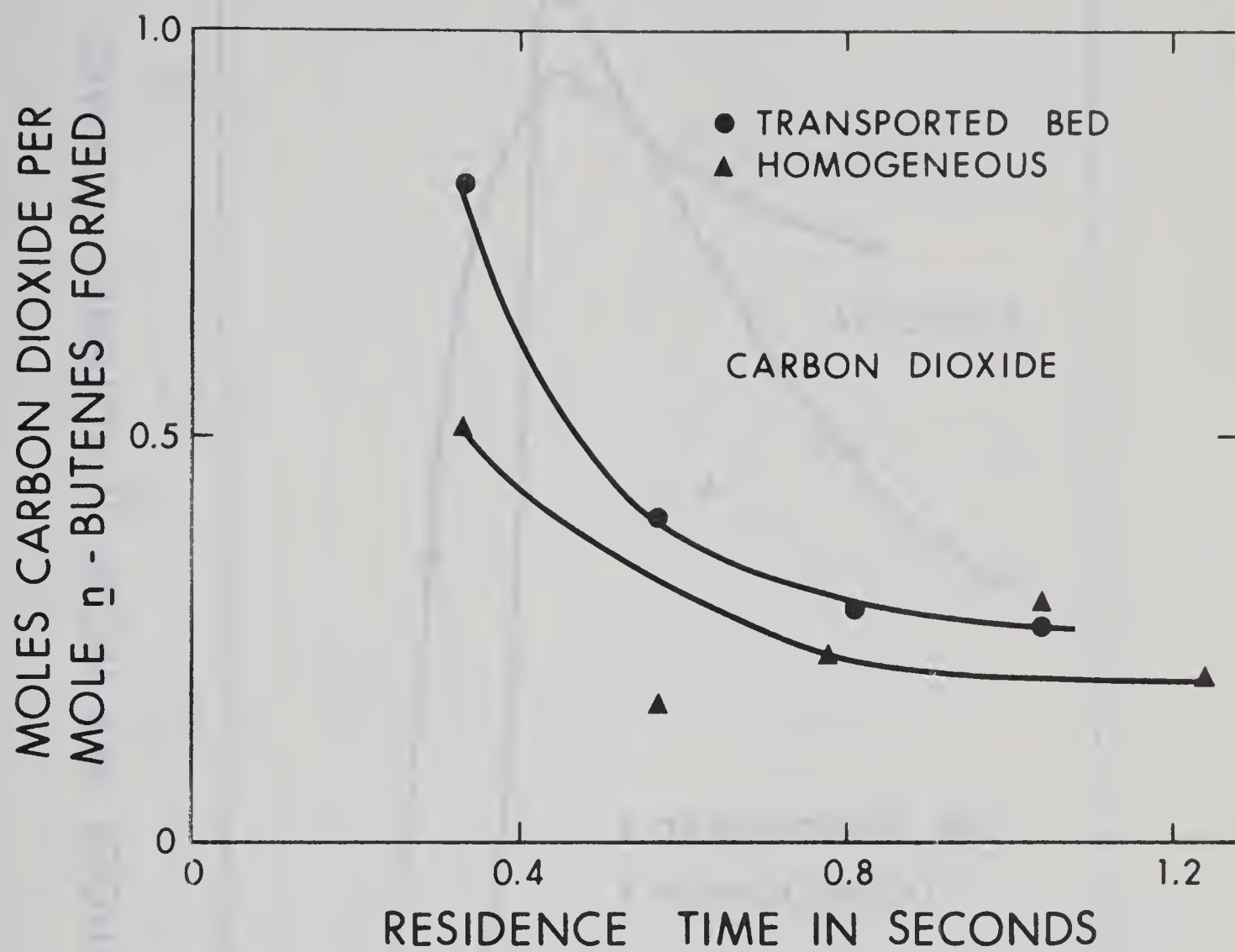


FIGURE 7.13 RELATIVE YIELD - EFFECT OF SURFACE

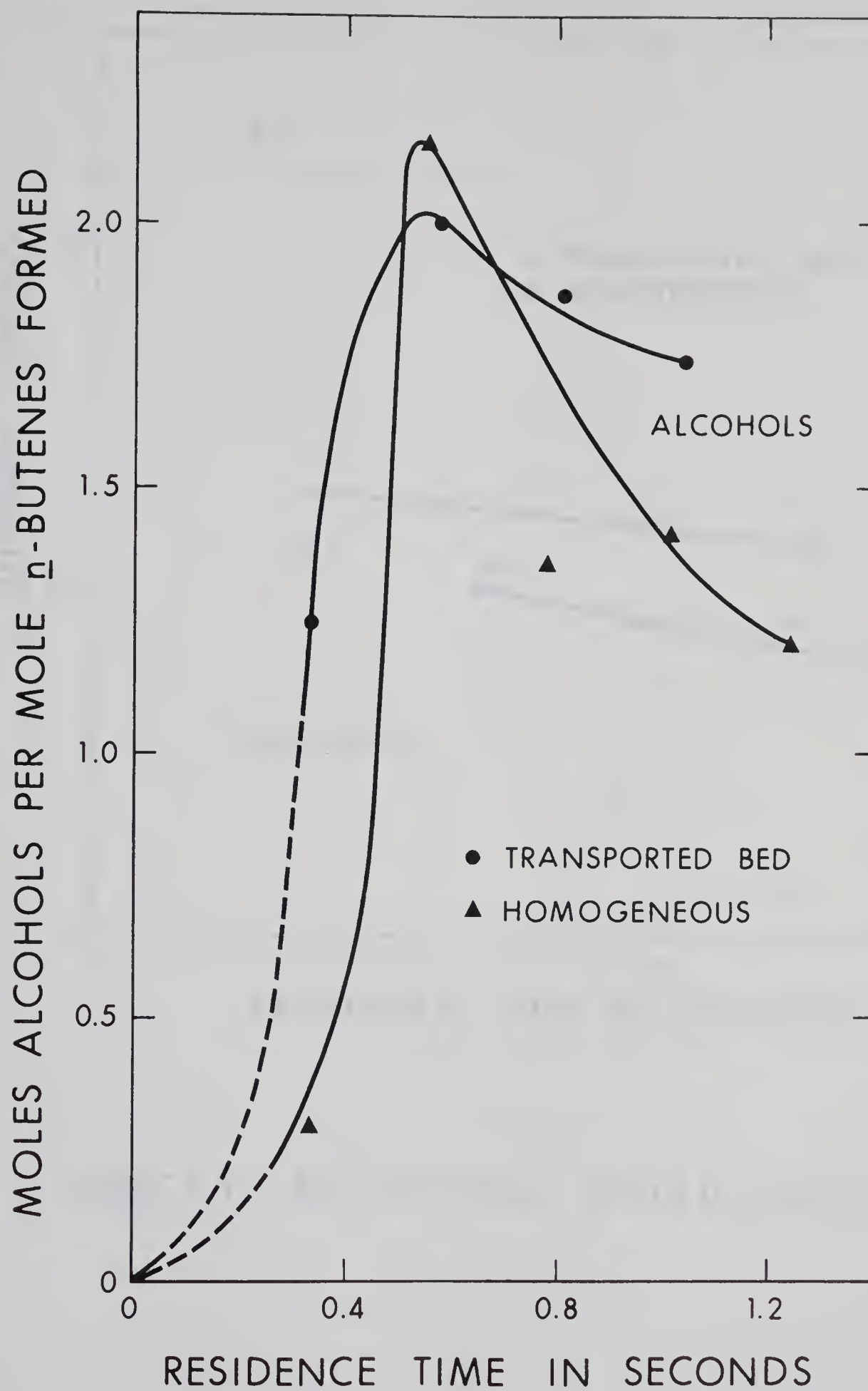


FIGURE 7.14 RELATIVE YIELD - EFFECT OF SURFACE

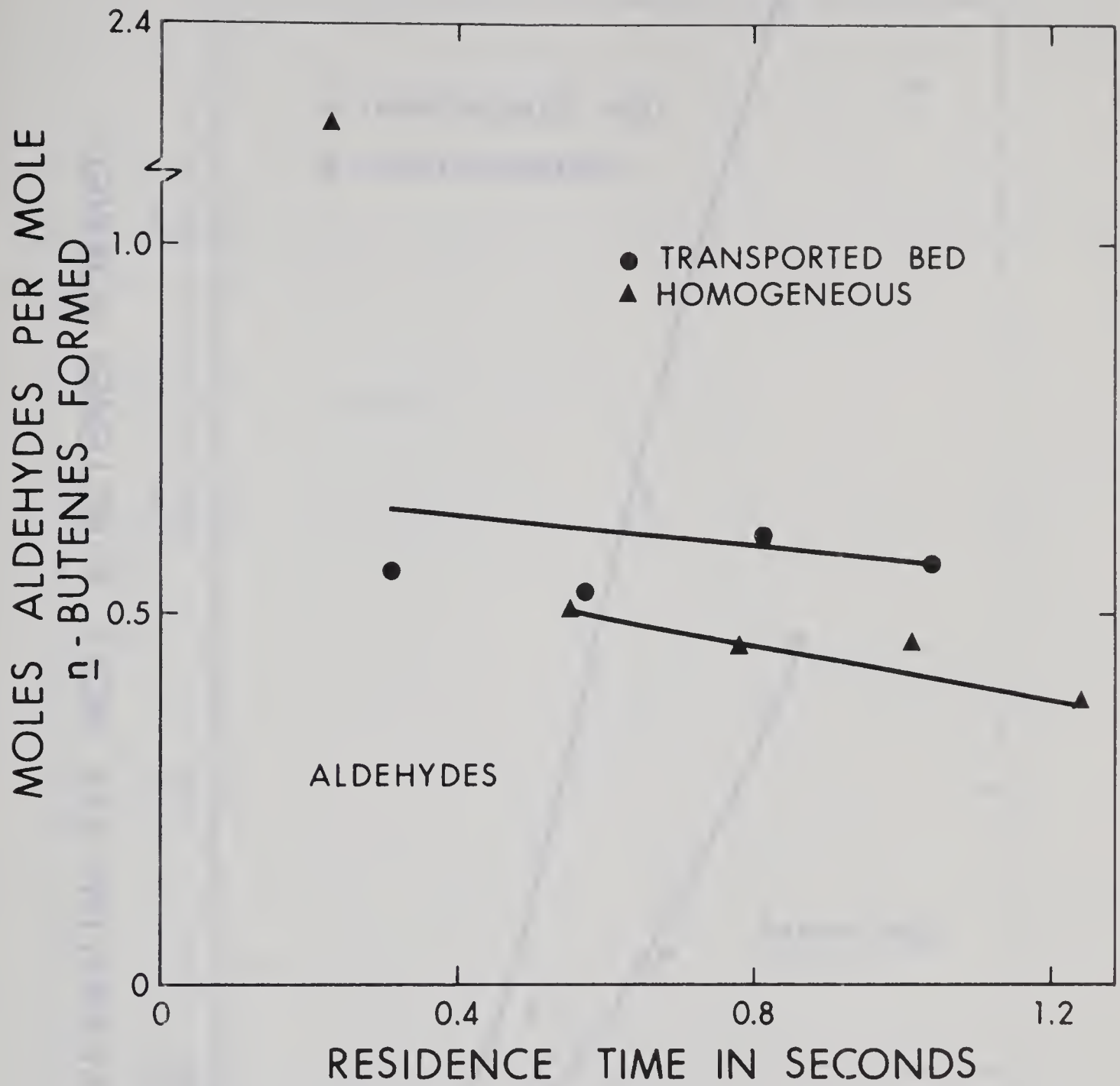


FIGURE 7.15 RELATIVE YIELD - EFFECT OF SURFACE

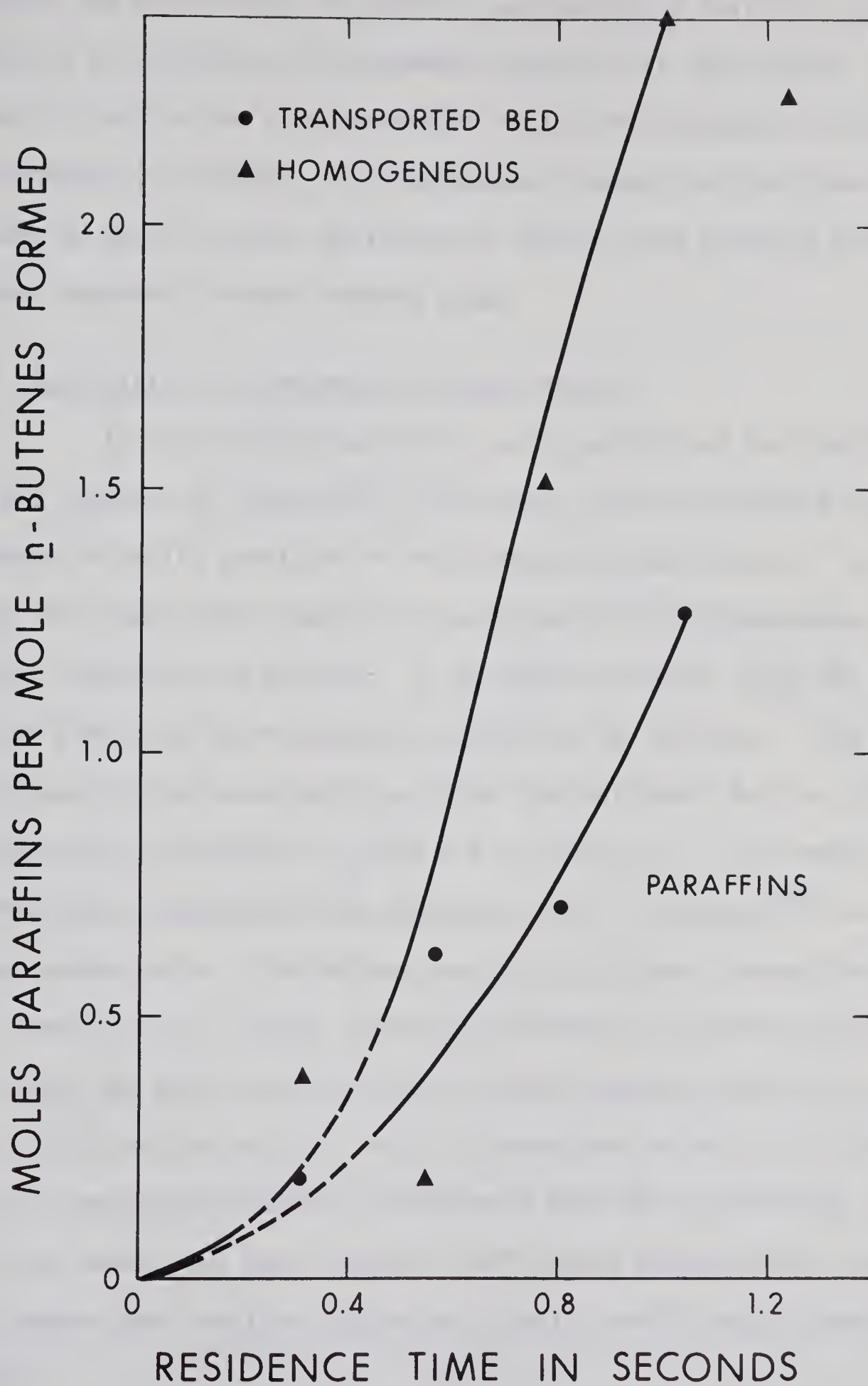


FIGURE 7.16 RELATIVE YIELD - EFFECT OF SURFACE

support the observations by Knox⁽¹⁸⁾ who suggested that the oxygenated products are formed by heterogeneous reactions at the surface. It is possible that in the slow combustion region investigated by Knox at subatmospheric pressure, the homogeneous propagation steps were slow enough to permit radical diffusion to the wall and reaction thereon to become important product forming steps.

7.4 Application of Homogeneous Kinetic Models

In the previous section it was hypothesized that the mechanisms of the reaction of hydrocarbon with oxygen remains unaltered by the presence of solid particles in the transported bed reactor. In that case, the same kinetic models as postulated for the homogeneous reactor could, therefore, be applied. It was found, however, that the models always predicted lower temperature profiles for the gas. This was attributed to the uncertainties in the thermal model for the system represented by equations 7.3 and 7.4 in section 7.2. The heat transfer coefficients calculated from equations in the literature⁽⁶⁹⁾ may be in considerable error. Preliminary runs with the model showed that it was not sensitive to a change in the heat transfer coefficient from gas to wall, but was quite sensitive to the heat transfer coefficient between the solids and the gas, h_c . With a correction factor of 0.8, the predicted temperature profiles matched well with the experimental profiles. In other words, the heat transfer coefficients determine the level of the temperature profiles, while the kinetic coefficients determine their shape.

The results after this modification are presented in Table 6.7. It is found that mechanism II predicts the overall conversions for n-butane and oxygen and the temperature profiles quite well. This is in

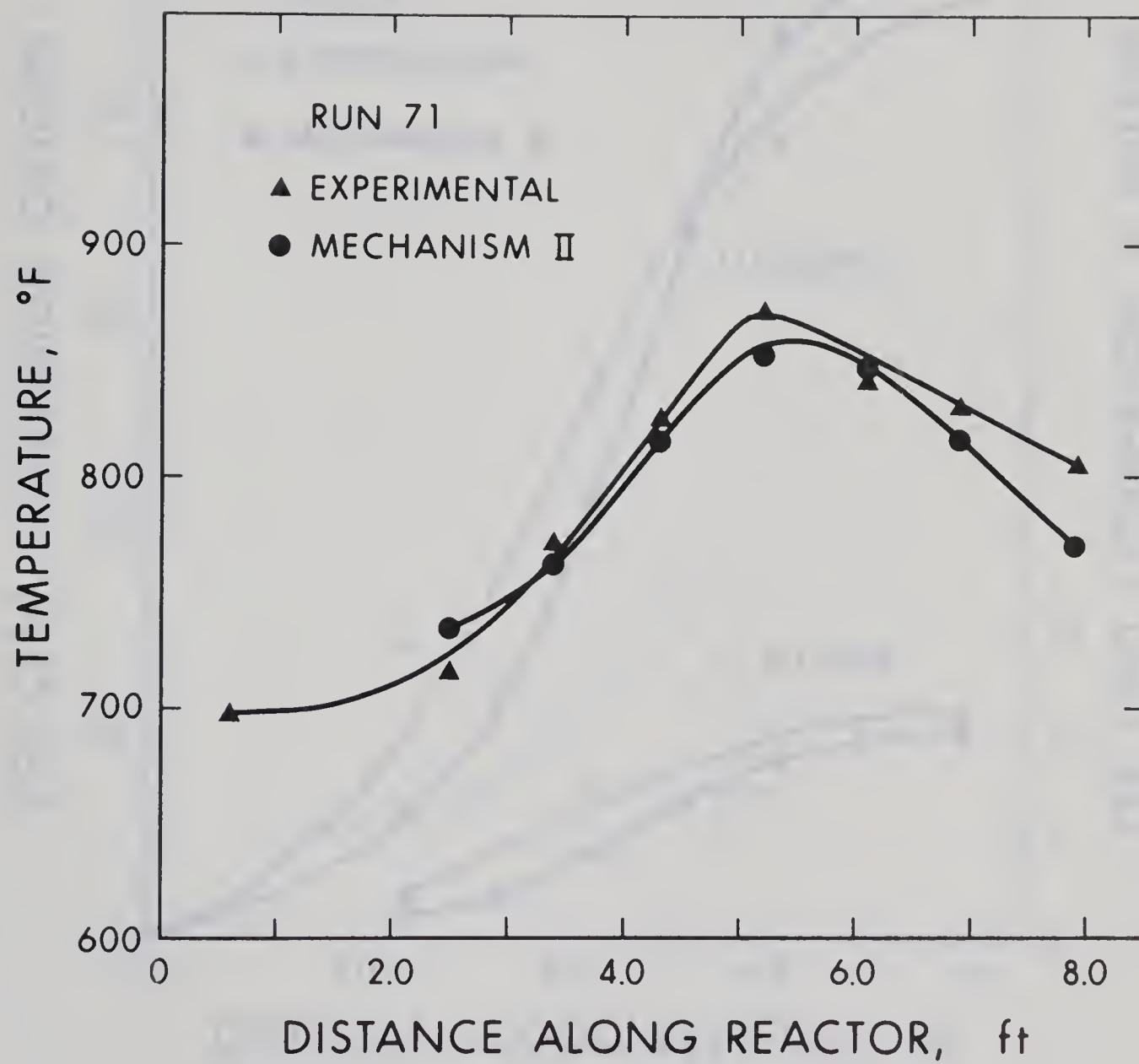


FIGURE 7.17 EXPERIMENTAL AND PREDICTED TEMPERATURE PROFILES

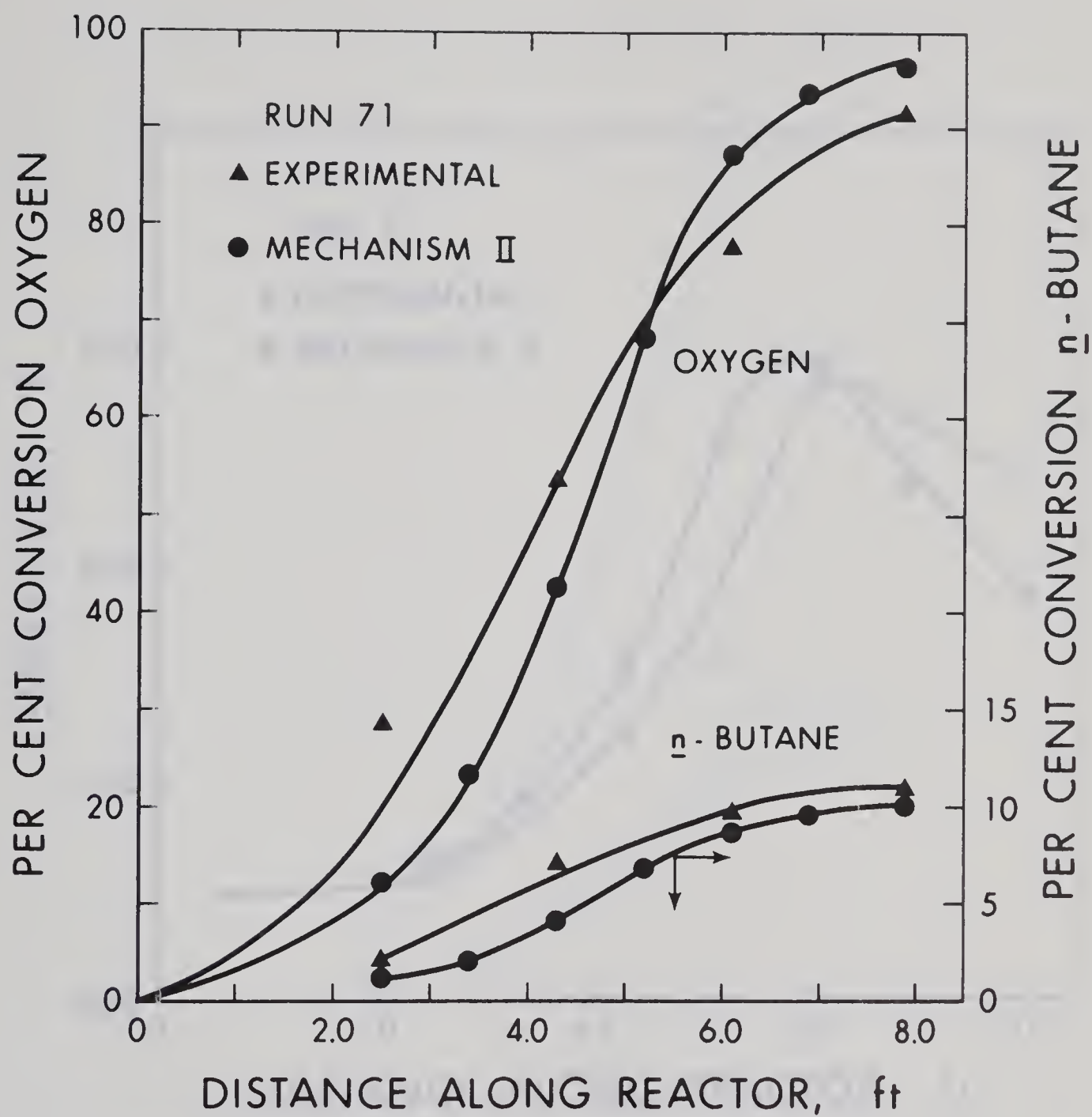


FIGURE 7.18 EXPERIMENTAL AND PREDICTED CONVERSIONS

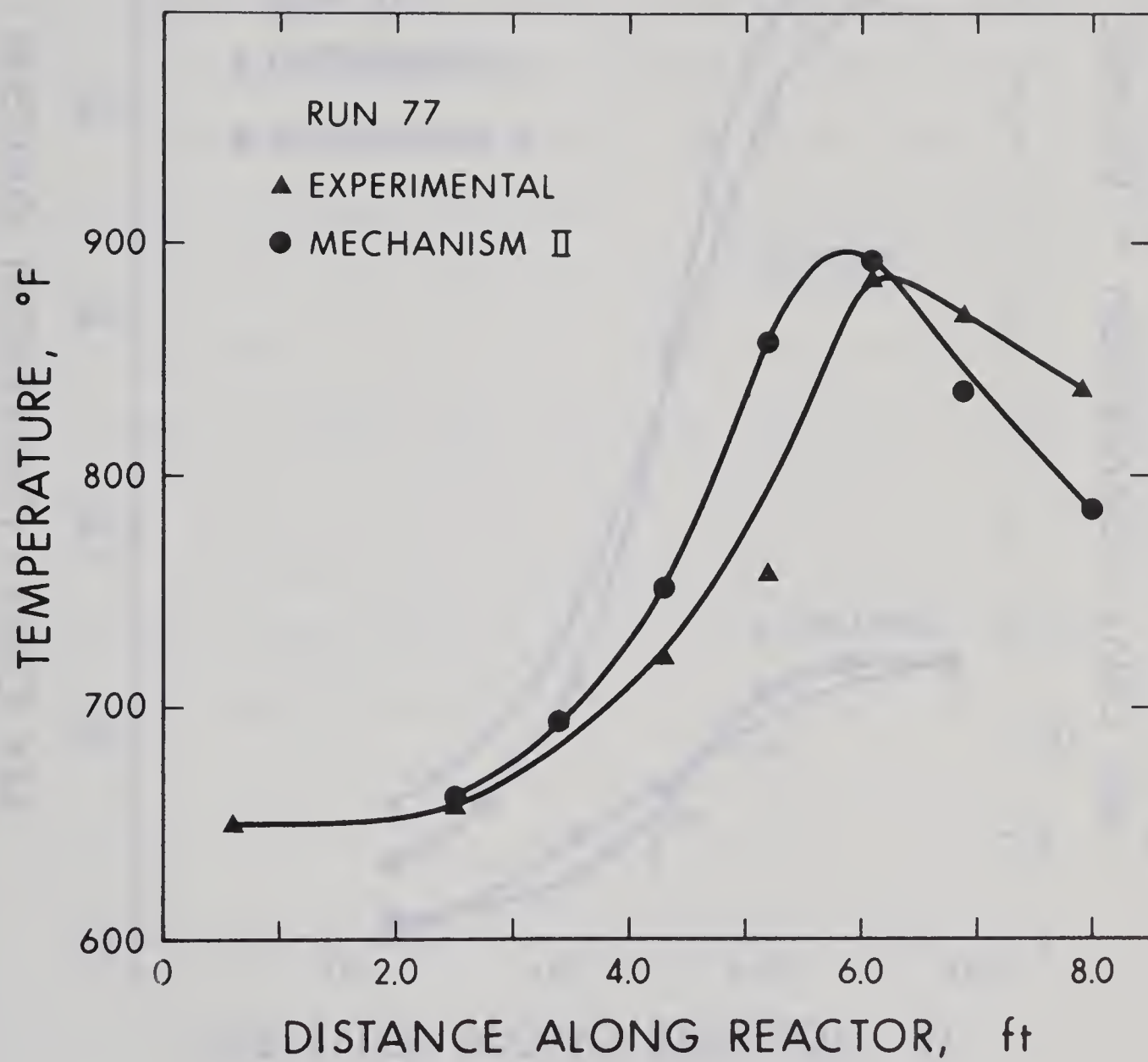


FIGURE 7.19 EXPERIMENTAL AND PREDICTED TEMPERATURE PROFILES

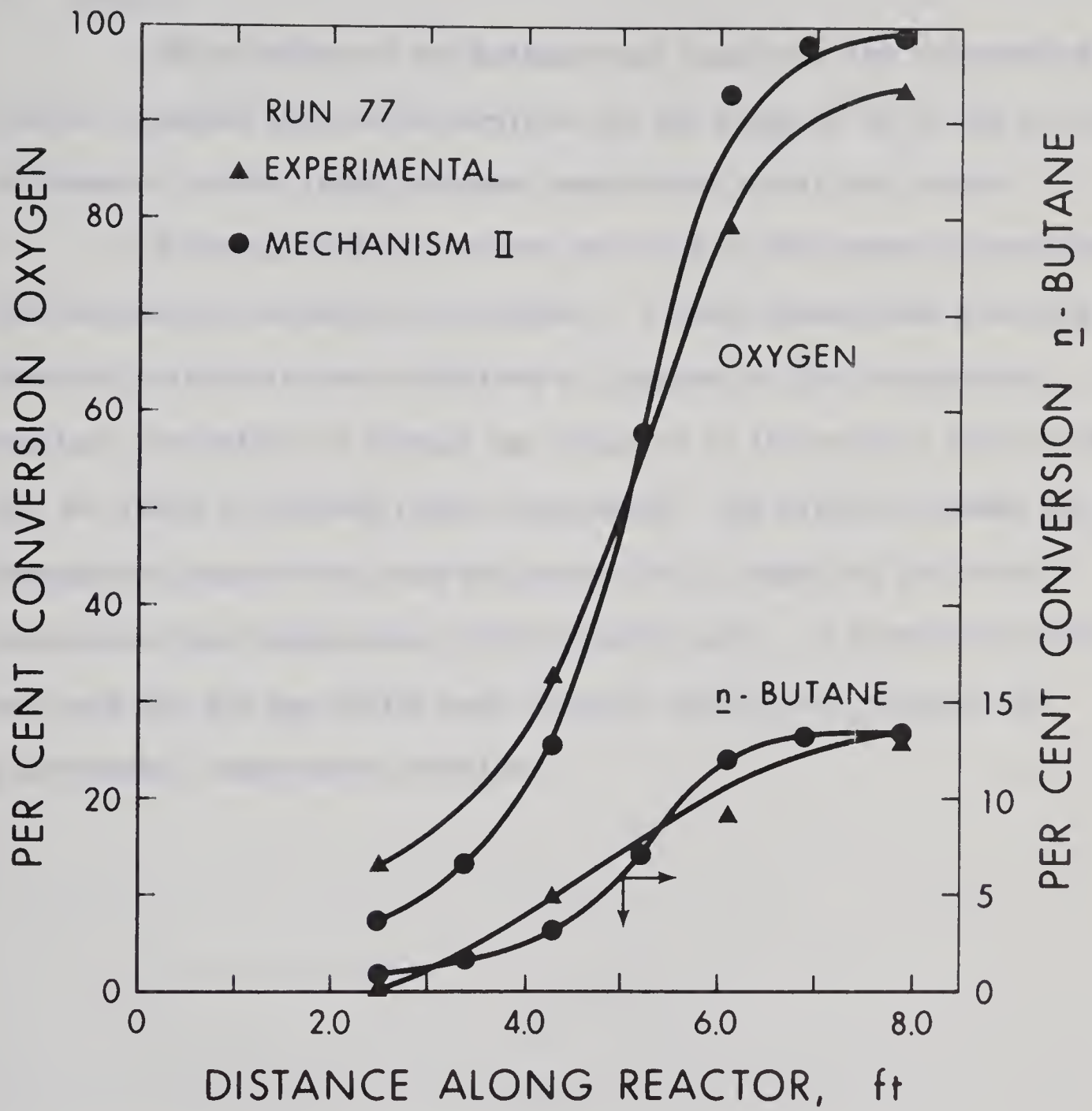


FIGURE 7.20 EXPERIMENTAL AND PREDICTED CONVERSIONS

accord with the results for the homogeneous runs in which case also model II is better. Figures 7.17 to 7.20 show the predicted and experimental temperature profiles and conversions for runs 71 and 77.

7.5 Summary

The solution of the mathematical model for the transported bed reactor revealed that solid particles of the range of up to 800 microns in diameter attain almost uniform temperature across the radius.

A transported bed reactor was used in the present investigation for the partial oxidation of n-butane. A lower temperature rise and an improved selectivity were obtained as compared to the homogeneous reactor. No effect of surface was observed on the product distribution for the range of loading ratios considered. The kinetic schemes for the homogeneous reactor was used and mechanism II predicted the overall conversions and temperature profiles fairly well. A correction factor was used for the gas solids heat transfer coefficient to match the experimental temperature profiles.

CHAPTER VIII

CONCLUSIONS AND RECOMMENDATIONS

8.1 Conclusions

A transported bed reactor system was developed which allowed a method of temperature control by the use of solid particles without having any undesirable effect on the overall reaction and product distribution. The maximum temperature rise was cut down by 150F° and the selectivity to oxygenated products was almost doubled compared to a similar run in a homogeneous reactor. The length of time for the rapid reaction was increased and the monitoring of the progress of the reaction was made easier.

The overall behaviour of the reaction was studied in the homogeneous reactor. Higher hydrocarbon to oxygen ratio was found to be beneficial to the formation of the oxygenated compounds. The inlet temperature did not influence the overall course of the reaction.

The homogeneous runs allowed the development of an aggregate model for the reaction. Two kinetic schemes were postulated for the homogeneous reaction and their parameters estimated. The models were tested against independent runs. The same kinetic models with modifications of the thermal parameters could successfully predict the overall conversions and temperature profiles for the transported bed reactor.

8.2 Recommendations

The use of the transported bed reactor provides an effective means of controlling the temperature rise without inhibition of the reaction. It may now be possible to use artificial initiator and start the reaction at a low temperature and continue the reaction at the lower

temperature level. This method is likely to improve the selectivity very significantly.

The range of investigation in the transported bed system can be increased by increasing the capacity of the solids feeder. This should be done by cutting deeper slots in the existing rotor. The solids heating system was inadequate, as the solids could not be heated beyond 650°F. A more compact solids heating unit should be built to replace the existing one.

NOMENCLATURE

A	Pre-exponential factor, normalized
A'	Pre-exponential factor, hr^{-1} or $\text{ft}^3/\text{lb-mole/hr}$
A_r	Cross-sectional area, ft^2
A_s	Solids surface area, ft^2/ft
A_w	Surface area of reactor wall, ft^2/ft
C	Specific heat of gas, $\text{Btu/lb/}^\circ\text{F}$
C_A	Concentration of <u>n</u> -Butane, lb-mole/ft^3
C_B	Concentration of Oxygen, lb-mole/ft^3
C_C	Concentration of intermediate, lb-mole/ft^3
C_D	Drag coefficient, dimensionless
C_p	Specific heat of solid particles, $\text{Btu/lb/}^\circ\text{F}$
D_r	Diameter of reactor, ft
d_p	Diameter of solid particles, ft
E	Activation energy, Btu/lb-mole
f	Friction factor, dimensionless
G_g	Gas flow rate, lb-mole/hr
G_o	Inlet gas flow rate, lb-mole/hr
g_c	Gravitational constant, $\text{lb}_m\text{ft/lb}_f\text{sec}^2$
h_c	Gas to solids heat transfer coefficient, $\text{Btu/hr/ft}^2/^\circ\text{F}$
h_w	Gas to wall heat transfer coefficient, $\text{Btu/hr/ft}^2/^\circ\text{F}$
ΔH	Heat of reaction, Btu/lb-mole
K	Reaction rate constant, hr^{-1} or $\text{ft}^3/\text{lb-mole/hr}$
K_s	Thermal conductivity of solids, $\text{Btu/hr/ft}^2\text{-ft/}^\circ\text{R}$
m	Gas flow rate, lb/hr
m_p	Solids to gas loading ratio, dimensionless

NOMENCLATURE (continued)

m_p^*	Initial solids to gas loading ratio, dimensionless
N	Number of solid particles/ft reactor, ft^{-1}
P	Pressure, lb/in^2
Q_g	Gas phase heat transfer, Btu
Q_s	Solids phase heat transfer, Btu
R	Universal gas constant, $\text{ft-lb/lb/}^\circ\text{F}$ or $\text{Btu/lb-mole/}^\circ\text{R}$
R_p	Particle Radius, ft
r	Reaction rate, lb-mole/hr/ft^3
r_p	Particle radius, ft
T	Gas temperature, $^\circ\text{R}$
T_p	Mean particle temperature, $^\circ\text{R}$
t	Time, hour
u	Velocity of gas, ft/sec
u_p	Velocity of particle, ft/sec
v	Temperature of solid particles, $^\circ\text{R}$
v_s	Surface temperature of solid particles, $^\circ\text{R}$
v	Specific volume of gas, ft^3/lb
w_p	Solids flow rate, lb/hr
x_A	Conversion of Butane, dimensionless
x_B	Conversion of Oxygen, dimensionless
x_C	Accumulation of intermediate, dimensionless
y_O	Inlet molar composition, fraction
Z	Distance along reactor, ft
α	Thermal diffusivity, ft^2/hr
ϵ	Void fraction, dimensionless

NOMENCLATURE (continued)

ρ	Gas density, lb/ft ³
ρ_p	Solids density, lb/ft ³
ρ_{ps}	Particulate phase density, lb/ft ³
τ	Time increment, hour
θ	Reduced time, dimensionless
μ	Viscosity of gas, lb/ft/hr

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APPENDIX A
EQUIPMENT DETAILS

The thermocouple and sample point locations are given in Table A.1. The temperature that the thermocouple measures is indicated by "G" if the thermocouple is in the gas stream, and by "W" if it is in the reactor wall. The location of the preheater and reactor control thermocouple is also indicated.

The properties of the solid particles and some of the equipment details are also presented.

TABLE A.1

Location of Thermocouples and Sample Points

Thermocouple Number	Temperature Measured	Location: Inches From Mixing Point	Sample Number
1	G	30.4	1
2	W	30.4	
3	G	41.1	
4	G	51.8	2
5	W	51.8	
6	G	62.5	
7	G	73.2	3
8	W	73.2	
9	G	83.9	
10	G	94.6	4
11	W	94.6	
12	G	105.3	
13	G	116.0	5
14	W	116.0	
15	Preheater		
16	Reactor	51.8	

Solid Particles

Material: Norton Crystalon (Silicon Carbide grain)

Physical Properties:

Size: 150 mesh

Crystal form: hexagonal system - hemihedral class

Melting temperature: dissociates at about 4170°F

True specific gravity: 3.20

Thermal conductivity at 800°F: 175 Btu/hr/ft²-in/°F

Specific heat at 750°F: 0.277 Btu/lb/°F

Chemical Properties:

General resistance to chemical action: high

Resistance to air oxidation: up to 2900°F

Typical Analysis:

Component	weight per cent
SiC	97.6
SiO ₂ (free)	0.8
Si (free)	0.5
C (free)	0.6
Fe	0.2
Al	0.2
Ca	0.05
Mg	<u>0.05</u>
	100.00

Electric Heaters

Solids Preheater:

Heating elements: Nikrothal 80 wire B & S 11

No. of elements: 14 elements in series

Inside diameter of heaters: 9.0 inches

Outside diameter: 11.5 inches

Maximum rating: 2.78 kw

Maximum current: 40 amps

Maximum voltage: 208 volts

Arrangement: 3 heaters in parallel

Gas Preheater:

Kanthal heaters

Heating length: 19.7 inches

Inside diameter: 5.0 inches

Outside diameter: 6.5 inches

Maximum rating: 5.873 kw

Maximum current: 55 amps

Maximum voltage: 107 volts

Arrangement: 2 heaters in series

Reactor heater:

Kanthal heaters

Heating length: 19.70 inches

Inside diameter: 1.57 inches

Outside diameter: 2.58 inches

Maximum rating: 1350 watts

Maximum voltage: 30 volts

Maximum current: 45 amps

Arrangement: 5 heaters in series

Control Systems

Pressure Controller:

Foxboro Model 58 P4 pneumatic controller

Pressure transmitter:

Foxboro M144 pressure transmitter

Control Valves:

Foxboro Type V4 needle valve, body size 1/2 inch, needle size 1/8 inch ($c_v = 0.07$) for air flow.

For n-butane flow, the same except needle size 0.024 inch ($c_v = 0.0052$).

For back pressure valve at reactor exit, needle size 3/16 inch ($c_v = 0.28$).

Flow Controllers:

For air and n-butane flow controls, Foxboro Model 58 Universal Pneumatic Controller.

Temperature Controllers:

For gas and solid preheaters, Foxboro Model 62 Universal Electronic Controller. The final control element is a Vectrol VS6002 Silicontrol Gate Drive. For reactor, Honeywell controller model R7161J. Model R4205A SCR power module provides solid state switching to the heaters.

APPENDIX B
RETENTION TIMES FOR THE COMPONENTS SEPARATED
BY GAS CHROMATOGRAPHY
SAMPLE CHROMATOGRAMS

The retention times for all the components separated on each column are given in Tables B.1 and B.2. The relative response factors and the correction factors are also included. Correction factors are not reported for the Molecular Sieve-Charcoal column, because this column is operated at constant temperature. The component numbers, given for all components, are used in Appendix E for the compounds reported in the analysis and product distributions.

Sample chromatograms are shown in order to indicate the degree of separation obtained in each column. The components separated and the attenuation for each peak are given on the chromatograms.

TABLE B.1

Retention Times for Components Separated

On Porapak S Column

Component Number	Component	Retention Time mins	Relative Response Factor	Correction Factor
1	Hydrogen	1.5	0.0085	1.0
2	Oxygen	1.5	0.40	1.0
3	Nitrogen	1.5	0.42	1.0
4	Carbon monoxide	1.8	0.42	1.0
5	Methane	2.5	0.36	1.0
6	Ethylene	5.5	0.48	1.0
7	Ethane	7.0	0.51	1.0
8	Propylene	16.4	0.63	1.04
9	Propane	17.0	0.65	1.04
10	<u>i</u> -Butane	22.9	0.82	1.03
11	1-Butene	21.6	0.81	1.04
12	2-Butene	23.6	0.86	1.03
13	<u>n</u> -Butane	24.2	0.85	1.05
14	2-Methyl Butane	37.2	1.05	1.05
15	<u>n</u> -Pentane	38.0	1.05	1.06
16	Carbon dioxide	3.5	0.42	1.0
17	Water	14.5	0.31	1.02
18	Formaldehyde	15.4	0.58	1.03
19	Methanol	21.0	0.58	1.05
20	Acetaldehyde	26.2	0.69	1.05
21	Ethanol	31.5	0.74	1.06
22	Ethylene Oxide	32.7	0.68	1.06
23	Acetone	33.7	0.86	1.05
24	Propionaldehyde	34.5	0.80	1.04
25	Propylene Oxide	35.3	0.80	1.05
26	<u>n</u> -Propanol	38.7	0.83	1.10
27	Butyraldehyde	39.3	0.92	1.07
28	Methyl Ethyl Ketone	46.0	0.98	1.08

TABLE B.1 (continued)

29	Sec-Butanol	50.5	0.97	1.10
30	Diethyl Ketone	53.0	1.10	1.10

TABLE B.2

Retention Times for Components Separated On
Charcoal-Molecular Sieve Column

Component Number	Component	Retention Time mins	Relative Response Factor
1	Hydrogen	2.5	0.0085
2	Oxygen	4.5	0.40
3	Nitrogen	5.0	0.42
4	Carbon Monoxide	7.5	0.42
5	Methane	13.0	0.36

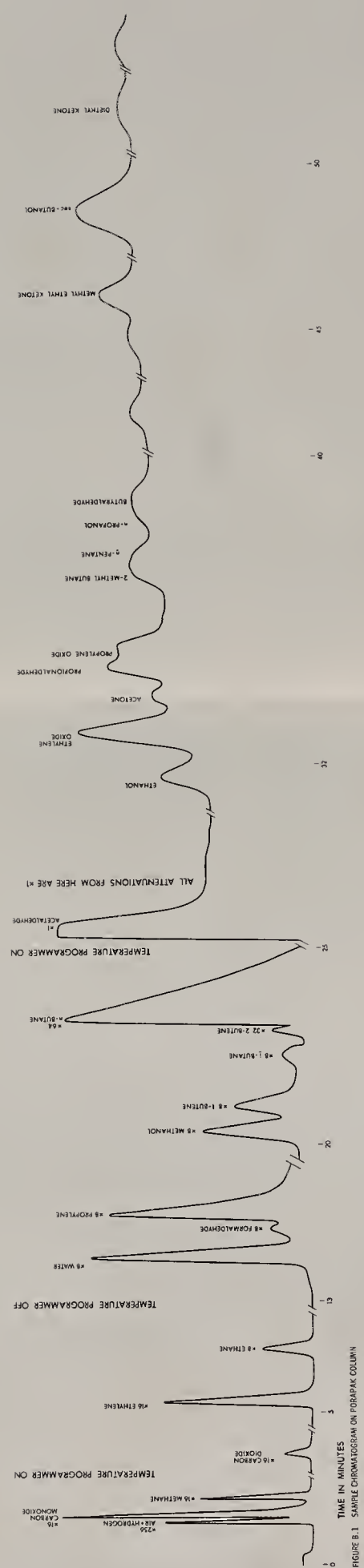


FIGURE B.1 SAMPLE CHROMATOGRAM ON PORAPAK COLUMN

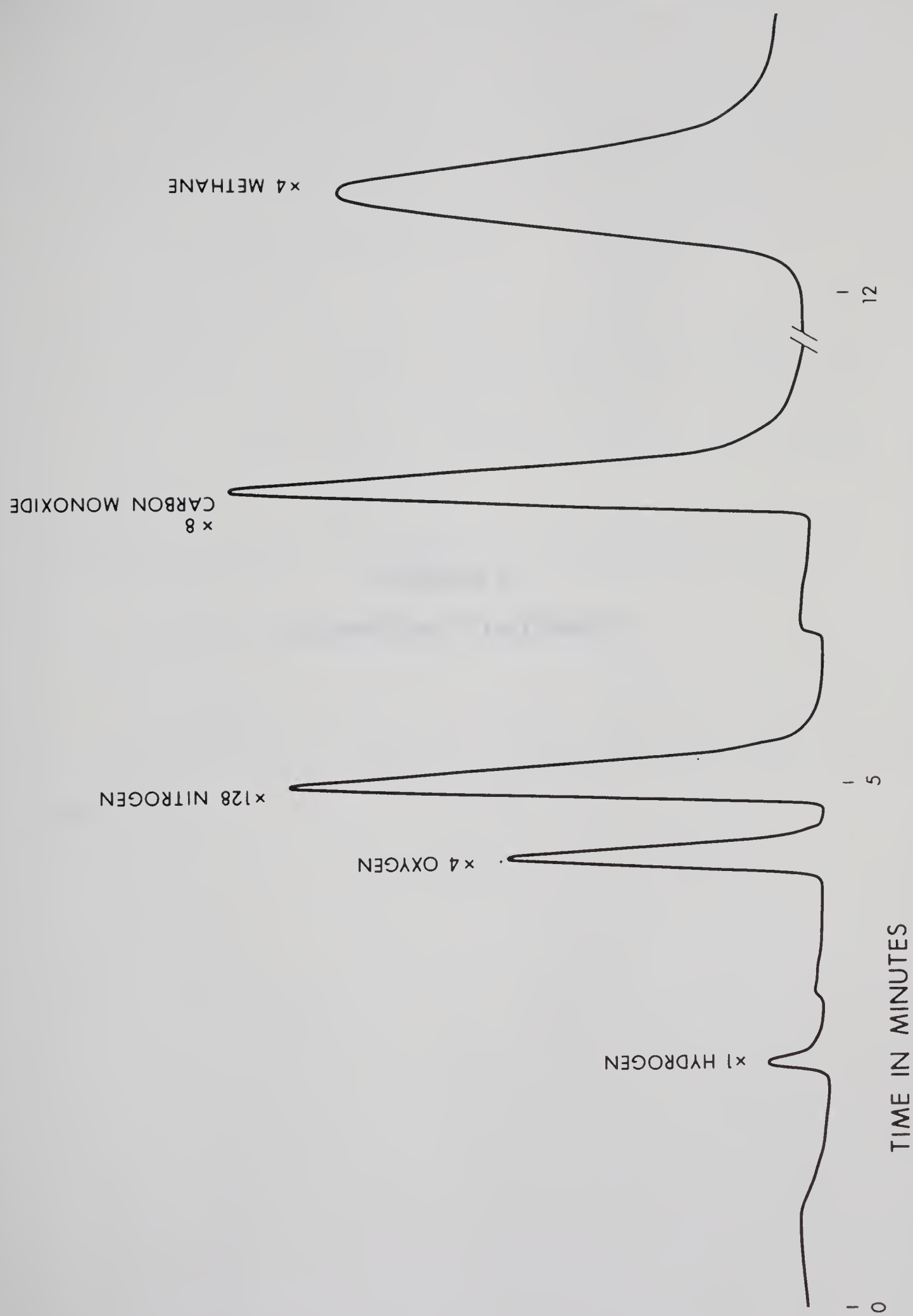


FIGURE B.2 SAMPLE CHROMATOGRAM ON MOLECULAR SIEVE-CHARCOAL COLUMN

APPENDIX C

CALIBRATION OF INSTRUMENTS

Calibration of Instruments

The D/P cells and the pressure transmitter were calibrated following standard procedures and the results are presented in Tables C.1, C.2 and C.3. The flow rates are plotted in Figures C.1 and C.2.

The D/P cell for n-butane was calibrated with water and then converted to n-butane by the formula given by Foxboro as:

$$\text{Equivalent water flow (gpm)} = V G_b \sqrt{\frac{1}{G_f}}$$

where V = flow of liquid n-butane in gpm at 60°F,

G_b = specific gravity of n-butane at 60°F,

G_f = specific gravity of n-butane at the flowing temperature.

Introduction of the proper values in the equation resulted in

$$n-C_4 \text{ (lb/hr)} = 0.755 \times \text{water (lb/hr)}$$

The calibration of the pressure transmitter is given in Table C.3. The calibration was found to be essentially exact over the entire range.

TABLE C.1

D/P Cell Calibration For Air

Orifice Diameter	0.0595 inches
D/P Cell Range	100 inches of water
Air Temperature	72°F
Atmospheric Pressure	698 mm Mercury

Controller Chart Reading per cent	Air Rate cu ft/min	Air Rate NTP cu ft/min	Air Rate lb/hr
35	0.51	0.434	2.10
65	0.705	0.598	2.90
82	0.776	0.66	3.20
49	0.606	0.515	2.50
55	0.655	0.556	2.70
40	0.564	0.478	2.32

TABLE C.2

D/P Cell Calibration for n-Butane

Orifice Diameter	0.02 inches
D/P Cell Range	250 inches of water
Water Temperature	70°F

Controller Chart Reading per cent	Water Rate lb/hr	<u>n</u> -Butane Rate lb/hr
41.4	10.52	7.95
59.4	12.68	9.56
21.9	7.39	5.57
79.6	14.8	11.18
90.4	15.81	11.95
34.2	9.36	7.07
51.9	11.82	8.94
41.4	10.38	7.84

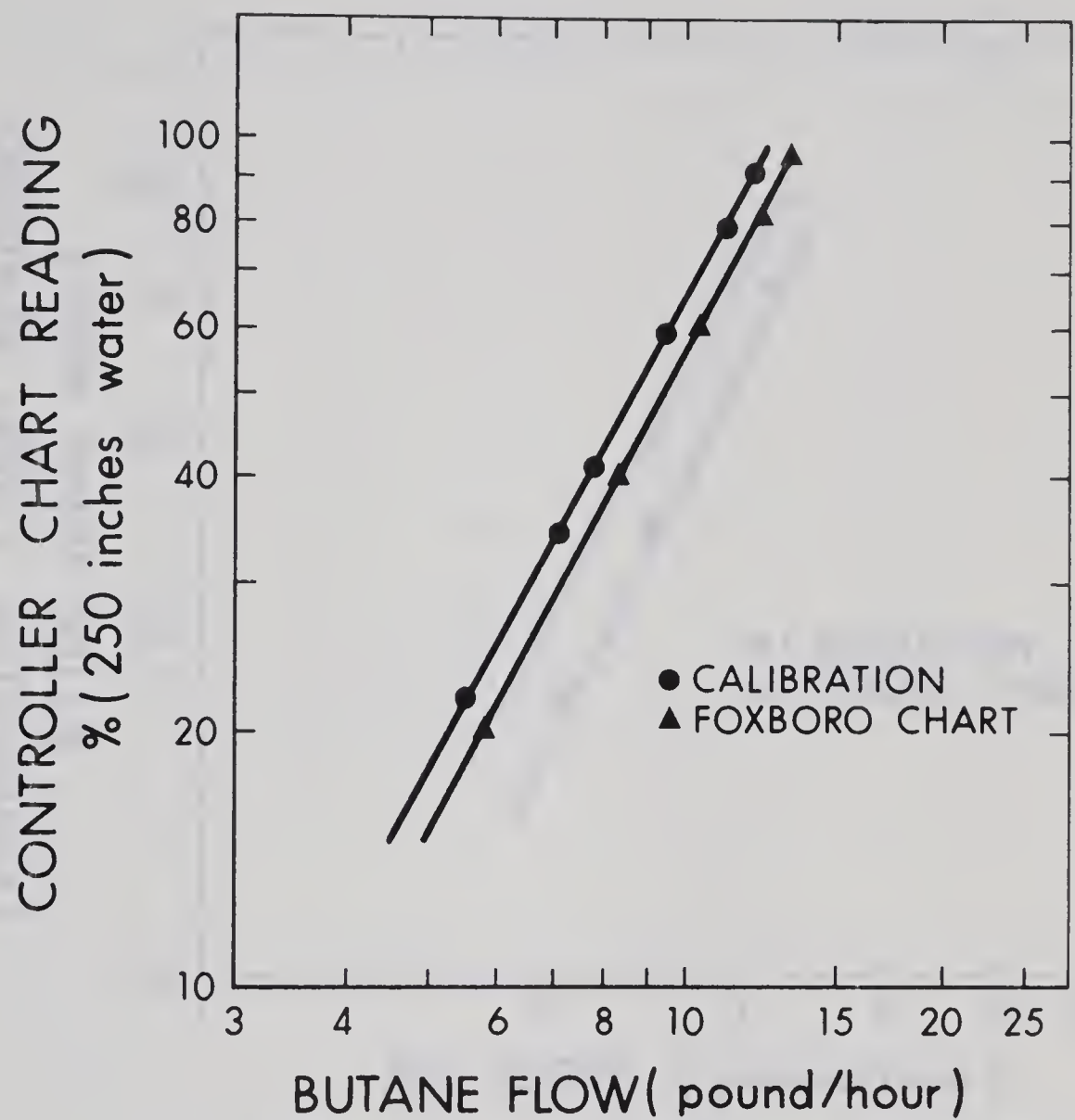


FIGURE C.1 CALIBRATION OF D/ P CELL

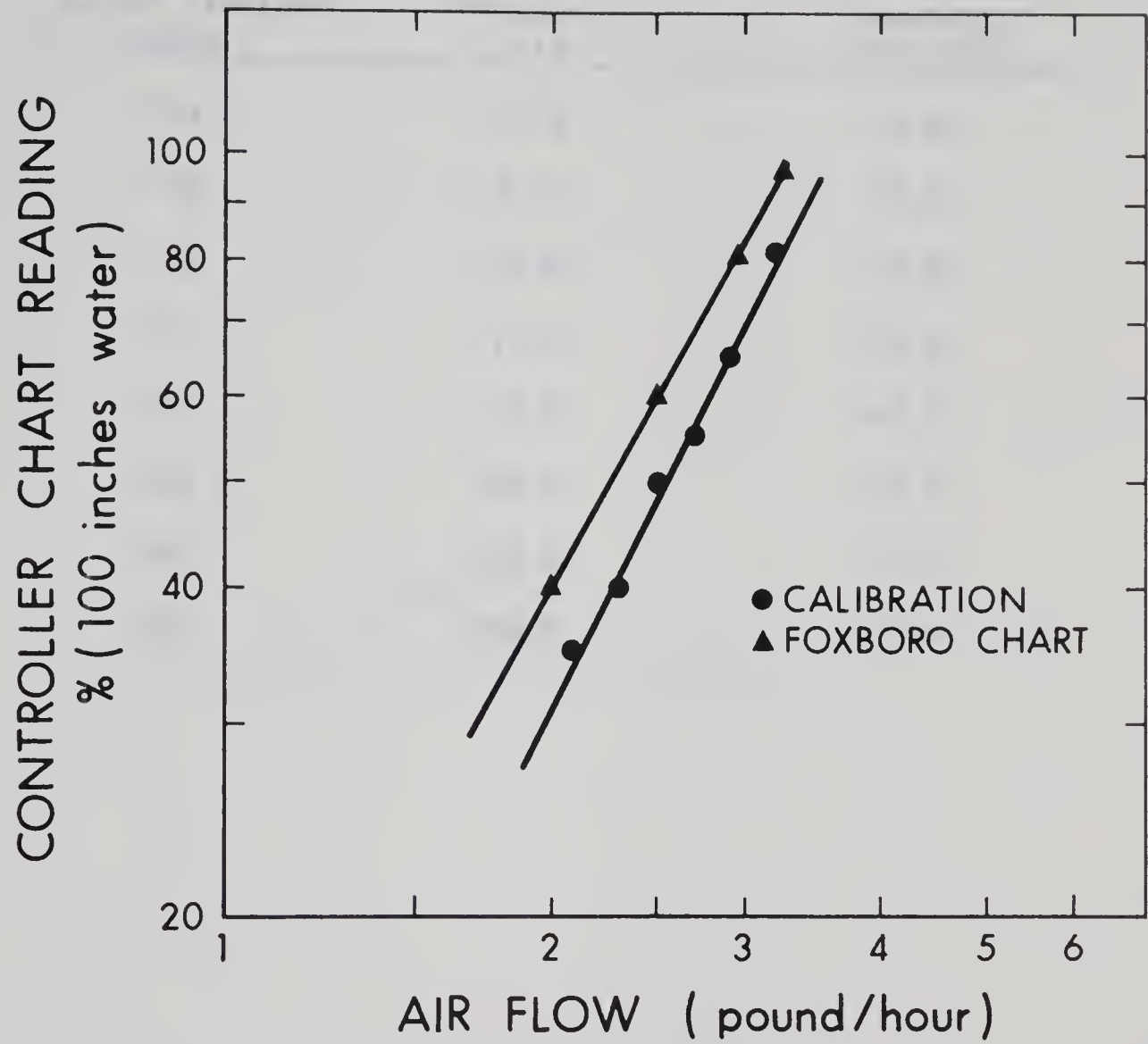


FIGURE C.2 CALIBRATION OF D/P CELL

TABLE C.3

Pressure Transmitter Calibration

Actual Pressure psig	Transmitter Pressure psig	Recorder Chart Reading per cent
20	20.0	10.0
40	40.0	20.0
50	50.0	25.0
70	70.0	35.0
80	80.0	40.0
100	100.0	50.0
150	150.0	75.0
200	200.0	100.0

The experimental temperatures for the homogeneous runs are presented in Table D.1 and those for the transported bed runs in Table D.2. All readings are the actual thermocouple recorded millivolts converted to degrees Fahrenheit. The errors due to conduction and radiation between the thermocouple and the reactor wall have been estimated to be about $12^{\circ}\text{F}^{(1)}$. Since the fluctuation in the temperature readings especially in the region of rapid reaction rate is much higher, no attempt has been made to correct for the radiation and conduction errors.

TABLE D.1
Experimental Temperature Profiles

Run Number	60	61	62	63	64	65	66	67	68
Thermocouple Number	Temperature °F								
15	685	695	695	702	692	687	708	684	684
1	658	666	672	684	666	672	705	667	672
2 w	660	667	672	689	670	690	727	698	692
3	655	678	676	696	670	679	830	705	685
4	700	737	705	820	714	790	1006	850	910
5 w	672	715	726	875	714	724	942	930	828
6	800	895	913	1041	825	1025	1040	1053	1004
7	915	950	970	1032	1025	1008	1002	971	915
8 w	804	810	852	912	870	889	896	820	828
9	870	910	932	997	1006	963	970	943	920
10	835	860	886	937	927	924	930	864	870
11 w	747	750	795	840	774	807	840	725	798
12	810	817	860	900	804	883	895	823	852
13	768	777	816	835	798	828	850	755	795
14 w	570	558	613	630		570	630		590

TABLE D.2
Experimental Temperature Profiles

Run Number	71	73	75	77	80
Thermocouple Number	Temperature °F				
15	698	678	655	650	625
1	715	650	648	660	655
2 w	740	668	665	692	750
3	770	660	650	695	705
4		690	680	722	800
5 w	805	730	715	830	850
6	872	740	692	758	900
7	842	800	735	885	885
8 w	740	770	710	755	805
9	830	830	775	870	875
10	805	860	805	838	850
11 w	670	730	695	660	740
12	770	840	810	810	825
13	730	800	785	755	795

APPENDIX E
EXPERIMENTAL RESULTS: HOMOGENEOUS AND
TRANSPORTED BED REACTORS

Reactor entrance conditions are calculated from the n-butane and air flow rates, the reactor pressure and the temperature at the entrance to the reactor. The calculation procedure is indicated below:

$$\text{Mole \% Oxygen} = 21 \left(\frac{\text{Air Flow Rate in lb moles/hr}}{\text{Total Flow Rate in lb moles/hr}} \right)$$

$$\text{Mole \% Nitrogen} = 79 \left(\frac{\text{Air Flow Rate in lb moles/hr}}{\text{Total Flow Rate in lb moles/hr}} \right)$$

$$\text{Mole \% } \underline{n}\text{-Butane} = 100 \left(\frac{\text{n-Butane Flow Rate in lb moles/hr}}{\text{Total Flow Rate in lb moles/hr}} \right)$$

$$\text{Ratio of } \frac{\text{Oxygen}}{\text{Nitrogen}} = \frac{\text{Mole \% Oxygen}}{\text{Mole \% Nitrogen}}$$

$$\text{Ratio of } \frac{\underline{n}\text{-Butane}}{\text{Nitrogen}} = \frac{\text{Mole \% } \underline{n}\text{-Butane}}{\text{Mole \% Nitrogen}}$$

$$\text{Density of the entering gas, } \rho_0 = \frac{mP}{RT}$$

$$\text{Entrance Velocity, } u_0 = \frac{w}{3600 A \rho_0}$$

$$\text{Residence Time, } \tau_0 = \frac{L}{u_0}$$

$$\text{Reynolds Number, } Re = \frac{D u_0 \rho_0}{\mu}$$

A = cross-sectional area of the reactor, ft²

D = inside diameter of reactor, ft

L = overall length of reactor, ft

m = average molecular weight of feed stream

P = reactor pressure, psia

R = gas constant

T = temperature of gases at entrance, °R

u_0 = velocity of gases at entrance, ft/sec

w = weight rate of flow of gases, lb/hr

ρ_0 = density of gases at entrance, lb/ft³

τ = residence time of the gases based on the entrance conditions, sec

μ = viscosity of gases at entrance, lb/ft.hr

For each product sample, the areas are converted to mole per cent by the use of the relative response factors and the correction factors. The procedure is as follows:

Calculate $\frac{\text{Component Area}}{\text{Relative Response Factor}}$ for each component or group of components on the Porapak S column and the Molecular Sieve-Charcoal column and find the total

$$TOT_{PR} = \sum \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

$$TOT_{MS-C} = \sum \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

Subscripts PR and MS-C refer to Porapak S and Molecular Sieve-Charcoal columns, respectively.

$$\% \text{ Component}_{PR} = \frac{100}{TOT_{PR}} \times \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

$$\% \text{ Component}_{MS-C} = \frac{100}{TOT_{MS-C}} \times \frac{\text{Component Area}}{\text{Relative Response Factor}}$$

The first peak in Porapak column contains hydrogen, oxygen and nitrogen. The first three peaks in Molecular Sieve-Charcoal column contain these components. Hence, their compositions can be obtained by multiplying the air peak by the proportions in which these components are present in Molecular Sieve-Charcoal column.

The percentage composition is converted to moles per mole nitrogen as follows:

$$\frac{\text{Moles Component}}{\text{Moles Nitrogen}} = \frac{\text{Mole \% Component}}{\text{Mole \% Nitrogen}}$$

A number of other calculations can now be made. The carbon, hydrogen and oxygen balances are made as follows:

$$\% \text{ Carbon Balance} = \frac{100 \times \sum \frac{\text{Moles Component}}{\text{Moles Nitrogen}} \times \text{No. of Carbon Atoms in Component}}{4 \times \sum \frac{\text{Moles n-Butane}}{\text{Moles Nitrogen}} \text{ in the feed}}$$

$$\% \text{ Hydrogen Balance} = \frac{100 \times \sum \frac{\text{Moles Component}}{\text{Moles Nitrogen}} \times \text{No. of Hydrogen Atoms in Component}}{10 \times \sum \frac{\text{Moles n-Butane}}{\text{Moles Nitrogen}} \text{ in the feed}}$$

$$\% \text{ Oxygen Balance} = \frac{100 \times \sum \frac{\text{Moles Component}}{\text{Moles Nitrogen}} \times \text{No. of Oxygen Atoms in Component}}{2 \times \sum \frac{\text{Moles Oxygen}}{\text{Moles Nitrogen}} \text{ in the feed}}$$

The per cent conversions of oxygen and n-butane can be found out.

$$\% \text{ Oxygen Reacted} = 100 \left(\frac{\frac{\text{Moles Oxygen}}{\text{Moles Nitrogen}} \text{ in the feed} - \frac{\text{Moles Oxygen}}{\text{Moles Nitrogen Product}}}{\frac{\text{Moles Oxygen}}{\text{Moles Nitrogen}} \text{ in the feed}} \right)$$

$$\% \text{ n-Butane Reacted} = 100 \left(\frac{\frac{\text{Moles n-Butane}}{\text{Moles Nitrogen}} \text{ in the feed} - \frac{\text{Moles n-Butane}}{\text{Moles Nitrogen Product}}}{\frac{\text{Moles n-Butane}}{\text{Moles Nitrogen}} \text{ in the feed}} \right)$$

The selectivities in terms of n-Butane and oxygen reacted are obtained as follows:

$$\frac{\text{Moles Component formed}}{\text{Mole Oxygen Reacted}} = \frac{\frac{\text{Moles Component formed}}{\text{Mole Nitrogen}}}{\frac{\text{Moles Oxygen Reacted}}{\text{Mole Nitrogen}}}$$

$$\frac{\text{Moles Component formed}}{\text{Mole } \underline{n}\text{-Butane Reacted}} = \frac{\frac{\text{Moles Component formed}}{\text{Mole Nitrogen}}}{\frac{\text{Moles } \underline{n}\text{-Butane Reacted}}{\text{Mole Nitrogen}}}$$

The per cent of carbon going to different types of products are calculated as follows:

$$\% \text{ Conversion to Olefins} =$$

$$100 \left(\frac{\frac{\text{Moles Olefins in the Product}}{\text{Mole } \underline{n}\text{-Butane Reacted}}}{\frac{\text{Moles Total Reaction Products}}{\text{Mole } \underline{n}\text{-Butane Reacted}}} \right)$$

Similar conversions to other groups of components are obtained in the same way.

The relative yield of different products can also be obtained from the selectivity calculations.

$$\frac{\text{Moles Components formed}}{\text{Mole } \underline{n}\text{-Butenes formed}} = \frac{\frac{\text{Moles Component formed}}{\text{Mole } \underline{n}\text{-Butane Reacted}}}{\frac{\text{Moles } \underline{n}\text{-Butenes formed}}{\text{Mole } \underline{n}\text{-Butane Reacted}}}$$

The yield relative to other components can be obtained similarly.

The computer program that was used in making these calculations is presented, followed by the results of all the experiments performed in this study.

C CHROMATOGRAPH

C CHROMATOGRAPH

C THIS PROGRAM TAKES IN THE INITIAL CONDITIONS FOR
 C THE REACTOR AND THE PEAK AREAS FOR THE PRODUCTS
 C FORM THE GAS CHROMATOGRAPHIC ANALYSIS. IT THEN
 C CALCULATES THE PRODUCT COMPOSITIONS AND SELEC-
 C TIVITIES, CONVERSIONS AND MATERIAL BALANCES.
 C

INTEGER PAGE

DIMENSION CAR(35),HYD(35),OXY(35),RSP(35),CRP(35)
 *,RSC(5),CRC(5)
 DIMENSION PRA(35),PRAM(35),PRAP(35),PRAPM(35),PCNT(35)
 *,PCNTM(35)
 DIMENSION CHA(5),CHAM(5),CHAP(5),CHAPM(5)
 DIMENSION CARB(35),RPN(35),HYDB(35),OXYB(35)
 *,RPTOX(35),RPTBT(35)

C NT NO. OF RUNS
 C NT NO. OF RUNS
 C NP NO. OF PEAKS IN PORAPAK COLUMN
 C NC NO. OF PEAKS IN CHARCOAL-MOLECULAR SIEVE
 C COLUMN
 C JP TOTAL NUMBER OF COMPONENTS PRESENT
 C NS NUMBER OF SAMPLES
 C RPT TOTAL MOLES PRODUCT PER MOLE BUTANE REACTED
 C OOXPR MOLE OXYGENATED PRODUCT/MOLE OXYGEN REACTED
 C OXPR MOLE CRACKING PRODUCT/MOLE OXYGEN REACTED
 C ORTN TOTAL MOLE OXYGENATED PRODUCT/MOLE NITROGEN
 C CRTN TOTAL MOLE CRACKING PRODUCT/MOLE NITROGEN
 C BOXPR MOLE OXYGENATED PRODUCT/MOLE BUTANE REACTED
 C CRPR MOLE CRACKING PRODUCT/MOLE BUTANE REACTED
 C RPT TOTAL MOLES PRODUCT PER MOLE BUTANE REACTED
 C

1 FORMAT(3F10.0)
 2 FORMAT(2F10.0)
 4 FORMAT(4F10.0)
 5 FORMAT(5F10.0)
 6 FORMAT(2I4)
 9 FORMAT(9I4)
 29 FORMAT(1H0,44X,5H E - ,I3/// 21X,9HRUN NO = ,I3,2X
 *,12HSAMPLE NO
 2= ,I2)
 32 FORMAT(1H0,21X,58HPRD NO MOL PERCENT MOLLS/MOL N2
 * MOLLS/MOXY R M
 20LS/MBUT R)
 38 FORMAT(1H0,21X,6HTOTALS,3(2X,F11.6)//18X,16HCARBON
 * BALANCE,F12.6
 2,13H LB AT/MOLN2.,F9.2,8H PERCENT/18X,17HHYDROGEN

CONTRACTS

[illegible]

WT	NO. OF RUNS
WT	NO. OF RUNS
NP	NO. OF PEAKS IN NMR SPECTRUM
NC	NO. OF PEAKS IN CHROMATOGRAM
COLMAN	
36	TOTAL NUMBER OF COMPONENTS DETECTED
42	NUMBER OF SAMPLES
WT	TOTAL MOLES PRODUCT PER MOLE BUTANE REACTANT
OXPH	MOLE OXYGENATED PRODUCT PER MOLE BUTANE REACTANT
OXPM	MOLE CRACKING PRODUCT PER MOLE BUTANE REACTANT
OXTH	TOTAL MOLE OXYGENATED PRODUCT PER MOLE BUTANE REACTANT
CTH	TOTAL MOLE CRACKING PRODUCT PER MOLE BUTANE REACTANT
OXMR	MOLE OXYGENATED PRODUCT PER MOLE BUTANE REACTANT
CTMR	MOLE CRACKING PRODUCT PER MOLE BUTANE REACTANT
PBT	TOTAL MOLES PRODUCT PER MOLE BUTANE REACTANT

[illegible]

C CHROMATOGRAPH ... (CONT'D)

```

* BALANCE ,F11.6,1
33H LB AT/MOLN2.,F9.2,8H PERCENT/18X,15HOXYGEN BALANCE
*,F13.6,13H L
4B AT/MOLN2., F9.2,8H PERCENT//18X,17HPERCENT O2 REACT
*,F10.4,4X,17
5HPERCENT C4 REACT ,F10.4)
50 FORMAT(1H0,      44X,5H E - ,I3/////21X,9HRUN NO = ,I3)
51 FORMAT( 1H0,20X,27HREACTOR ENTRANCE CONDITIONS //)
53 FORMAT(1H0,20X,6HAIR = ,F6.2,6H LB/HR,10X,9HBUTANE =
*,F6.2,6H LB/H
2R, //21X,14HTEMPERATURE = ,F8.2,7H DEG F ,//21X
*,11HPRESSURE = ,F6.2
3,9H LB/SQ IN, //21X,9HOXYGEN = ,F6.4,12H NITROGEN =
*,F7.4,10H BUTAN
4E = ,F7.4,1X,9H MOL PCNT//21X,8HOXY/N = ,F6.4,10H NIT
*/N = ,F6.4,1
50H BUT/N = ,F7.4,10H MOLS/MN2/)
54 FORMAT(21X,31HBUTANE TO OXYGEN MOLAR RATIO = ,F8.4/
*/21X,25HDENSITY
2 OF GAS MIXTURE = ,F8.4,9H LB/CU FT//21X,15HGAS
* VELOCITY = ,F6.2,7
3H FT/SEC //21X,47HRESIDENCE TIME BASED ON ENTRANCE
* CONDITIONS = ,
4F5.2,5H SEC //21X,18HREYNOLDS NUMBER = ,I7)
93 FORMAT(1H1)
107 FORMAT(1X,22X,I3,2X,4(2X,F11.6))
199 FORMAT(28X,30HMOLE PRODUCT PER MOLE N-BUTANE)
201 FORMAT(/ 20X,2HCO,6X,3HCO2,3X,5HBUTEN,3X,6HPARFIN,2X
*,6HALCOHL,2X,6
2HALDHYD,2X,6HOXYGCO,3X,5HWATER)
203 FORMAT(16X,10F8.4)
204 FORMAT(28X,31HMOLE PRODUCT PER MOLE N-BUTENES)
206 FORMAT(28X,24HMOLE PRODUCT PER MOLE CO)
208 FORMAT(28X,28HMOLE PRODUCT PER MOLE ETHENE)

```

PAGE=13

C READ IN THE CONSTANTS
C

```

READ(5,9)NP,NC,NJ,JP,NT
READ(5,1)(CAR(I),HYD(I),OXY(I),I=1,JP)
READ(5,2)(RSP(I),CRP(I),I=1,NP)
READ(5,2)(RSC(I),CRC(I),I=1,NC)
WRITE(6,93)
DO 75 LPN=1,NT
READ(5,6)NRUN,NS

```

C READ IN THE INPUT DATA

[illegible]
$$f_j = -3.0 \times 10^4$$

2700 2000 1000 0

[illegible]

C CHROMATOGRAPH ... (CONT'D)

C

```
READ(5,4)ARW,BTW,PR,TG
```

```
GSW=ARW+BTW
ARM=ARW/28.855
BTM=BTW/58.124
GSM=ARM+BTM
ARP=ARM/GSM*100.0
BTP=BTM/GSM*100.0
OXP=0.21*ARP
TNP=0.79*ARP
OTN=OXP/TNP
BTN=BTP/TNP
TTN=TNP/TNP
TNN=OTN+BTN+TTN
BTO=BTN/OTN
XAR=0.01*ARP
XBT=0.01*BTP
AVM=28.855*XAR+58.124*XBT
DG=AVM*PR/(10.73*(460.+TG))
VEL=GSW/(7.67*DG)
```

C
C

```
CALCULATE THE RESIDENCE TIMES
```

```
RES=9.75/VEL
RES=116.0/(12.0*VEL)
RES1=5.0/(12.0*VEL)
RES2=30.4/(12.0*VEL)
RES3=41.1/(12.0*VEL)
RES4=51.8/(12.0*VEL)
RES5=62.5/(12.0*VEL)
RES6=73.5/(12.0*VEL)
RES7=83.9/(12.0*VEL)
RES8=94.6/(12.0*VEL)
RES9=105.3/(12.0*VEL)
```

```
UAR=2.42*(0.0175+0.000019*TG)
UBT=2.42*(0.0063+0.0000134*TG)
UG=(5.372*XAR*UAR+7.624*XBT*UBT)/(5.372*XAR+7.624*XBT)
RN=187.5*VEL*DG/UG
IRN=RN
WRITE(6,50)PAGE,NRUN
WRITE(6,51)
WRITE(6,53)ARW,BTW,TG,PR,OXP,TNP,BTP,OTN,TTN,BTN
WRITE(6,54)BTO,DG,VEL,RES,IRN
WRITE(6,93)
```


C CHROMATOGRAPH ... (CONT'D)

```

DO 500 LJ=1,NS
READ(5,9)NSAMP
PAGE=PAGE+1
READ(5,5)(PRA(I),I=1,NP)
READ(5,5)(CHA(I),I=1,NC)
PRAS=0.0
PRASM=0.0
DO 10 I=1,NP
PRAM(I)=PRA(I)/RSP(I)/CRP(I)
PRAS=PRAS+PRA(I)
PRASM=PRASM+PRAM(I)
10 CONTINUE
PRAT=0.0
PRATM=0.0
DO 11 I=1,NP
PRAP(I)=PRA(I)/PRAS*100.0
PRAPM(I)=PRAM(I)/PRASM*100.0
PRAT=PRAT+PRAP(I)
PRATM=PRATM+PRAPM(I)
11 CONTINUE
CHAS=0.0
CHASM=0.0
DO 12 I=1,NC
CHAM(I)=CHA(I)/RSC(I)/CRC(I)
CHAS=CHAS+CHA(I)
CHASM=CHASM+CHAM(I)
12 CONTINUE

C      CALCULATE WT PER CENT AND MOL PER CENT
C
DO 13 I=1,NC
CHAP(I)=CHA(I)/CHAS*100.0
CHAPM(I)=CHAM(I)/CHASM*100.0
13 CONTINUE
TCNT=0.0
TCNTM=0.0
DO 14 I=1,NJ
PCNT(I)=CHAP(I)*PRAP(1)/100.0
PCNTM(I)=CHAPM(I)*PRAPM(1)/100.0
TCNT=TCNT+PCNT(I)
TCNTM=TCNTM+PCNTM(I)
14 CONTINUE
DO 15 I=2,NP
JK=NJ+I-1
PCNT(JK)=PRAP(I)
PCNTM(JK)=PRAPM(I)
TCNT=TCNT+PCNT(JK)
TCNTM=TCNTM+PCNTM(JK)
15 CONTINUE

```


C CHROMATOGRAPH ... (CONT'D)

C MAKE CARBON HYDROGEN AND OXYGEN BALANCES
C

```

TCARB=0.0
THYDB=0.0
TOXYB=0.0
TRPN=0.0
DO 26 I=1,JP
RPN(I)=PCNTM(I)/PCNTM(3)
CARB(I)=RPN(I)*CAR(I)
HYDB(I)=RPN(I)*HYD(I)
OXYB(I)=RPN(I)*OXY(I)
TCARB=TCARB+CARB(I)
THYDB=THYDB+HYDB(I)
TOXYB=TOXYB+OXYB(I)
TRPN=TRPN+RPN(I)
26 CONTINUE
PCARB=TCARB/(4.0*BTN)*100.0
POXYB=TOXYB/(2.0*OTN)*100.0
PHYDB=THYDB/(10.0*BTN)*100.0
OXRTN=(OTN-RPN(2))/OTN*100.0
BTRTN=(BTN-RPN(13))/BTN*100.0
OXRT=OTN-RPN(2)
BTRT=BTN-RPN(13)

```

C CALCULATE SELECTIVITIES
C
C PRODUCTS FORMED PER MOLE BUTANE AND
C OXYGEN REACTED
C

```

RPT=0.0
RPO=0.0
DO 27 I=1,JP
RPTOX(I)=RPN(I)/OXRT
RPTBT(I)=RPN(I)/BTRT
RPT=RPT+RPTBT(I)
RPO=RPO+RPTOX(I)
27 CONTINUE
WRITE(6,29)PAGE,NRUN,NSAMP
WRITE(6,32)
DO 73 I=1,JP
WRITE(6,107)I,PCNTM(I),RPN(I),RPTOX(I),RPTBT(I)
73 CONTINUE
WRITE(6,38)TCNT,TCNTM,TRPN,TCARB,PCARB,THYDB,PHYDB
*,TOXYB,POXYB,OXR
2TN,BTRTN
RPT=RPT-RPTBT(2)-RPTBT(3)-RPTBT(13)
RPO=RPO-RPTOX(2)-RPTOX(3)-RPTOX(13)

```


C CHROMATOGRAPH ... (CONT'D)

```

CRTN=0.0
ORTN=0.0
OOXPR=0.0
BOXPR=0.0
DO 71 I=18,JP
BOXPR=BOXPR+RPTBT(I)
OOXPR=OOXPR+RPTOX(I)
ORTN=ORTN+RPN(I)
71 CONTINUE
CRPR=0.0
OXPR=0.0
DO 72 I=5,15
CRPR=CRPR+RPTBT(I)
OXPR=OXPR+RPTOX(I)
CRTN=CRTN+RPN(I)
72 CONTINUE
CRPR=CRPR-RPTBT(13)+RPTBT(1)
OXPR=OXPR-RPTOX(13)+RPTOX(1)
CRTN=CRTN-RPN(13)+RPN(1)

```

C PER CENT N-BUTANE REACTED TO DIFFERENT PRODUCTS

```

COCO2=(RPTBT(4)+RPTBT(16))/RPT*100.0
OLEF=(RPTBT(6)+RPTBT(9)+RPTBT(11)+RPTBT(12))/RPT*100.0
PARL=(RPTBT(5)+RPTBT(7)+RPTBT(8))/RPT*100.0
H2O=RPTBT(17)/RPT*100.0
ALKET=RPTBT(23)+RPTBT(28)+RPTBT(30)
ALDE=RPTBT(18)+RPTBT(20)+RPTBT(24)+RPTBT(27)
ALCO=RPTBT(19)+RPTBT(21)+RPTBT(26)+RPTBT(29)
DEHYD=RPTBT(6)+RPTBT(9)+RPTBT(11)+RPTBT(12)
CRACK=RPTBT(5)+RPTBT(7)+RPTBT(8)+RPTBT(1)
OXYG=0.0
DO 79 KK=18,JP
OXYG=OXYG+RPTBT(KK)
79 CONTINUE
OXYGE=OXYG
OXYG=OXYG/RPT*100.0

```

```

BUTEN=RPTBT(11)+RPTBT(12)
CO=RPTBT(4)
CO2=RPTBT(16)
WATER=RPTBT(17)
X1=CRACK
X2=OXYGE
X3=ALCO
X4=ALDE
X5=ALKET
Y1=BUTEN

```

(1) $(\mathcal{L}_1, \mathcal{L}_2) \in \mathcal{L}(\mathcal{L}_1, \mathcal{L}_2)$ and $(\mathcal{L}_1, \mathcal{L}_2) \in \mathcal{L}(\mathcal{L}_1, \mathcal{L}_2)$.

C CHROMATOGRAPH ... (CONT'D)

Y2=DEHYD
 Y3=CO
 Y4=WATER
 Y5=RPTBT(6)
 WRITE(6,201)
 WRITE(6,199)
 WRITE(6,203)CO,CO2,BUTEN,CRACK,ALCO,ALDE,OXYGE,WATER

C MOLE PRODUCT PER MOLE BUTENES
C

CO=CO/Y1
 CO2=CO2/Y1
 BUTEN=BUTEN/Y1
 DEHYD=DEHYD/Y1
 CRACK=CRACK/Y1
 ALCO=ALCO/Y1
 ALDE=ALDE/Y1
 ALKET=ALKET/Y1
 OXYGE=OXYGE/Y1
 WATER=WATER/Y1
 WRITE(6,204)
 WRITE(6,203)CO,CO2,BUTEN,CRACK,ALCO,ALDE,OXYGE,WATER

C MOLE PRODUCT PER MOLE OLEFINS
C

CO=RPTBT(4)/Y2
 CO2=RPTBT(16)/Y2
 BUTEN=Y1/Y2
 DEHYD=Y2/Y2
 CRACK=X1/Y2
 ALCO=X3/Y2
 ALDE=X4/Y2
 ALKET=X5/Y2
 OXYGE=X2/Y2
 WATER=Y4/Y2

C MOLE PRODUCT PER MOLE CARBON MONOXIDE
C

CO=RPTBT(4)/Y3
 CO2=RPTBT(16)/Y3
 BUTEN=Y1/Y3
 DEHYD=Y2/Y3
 CRACK=X1/Y3
 ALCO=X3/Y3
 ALDE=X4/Y3
 ALKET=X5/Y3
 OXYGE=X2/Y3

$$1 \rightarrow \mathbb{Z} \rightarrow M \rightarrow 0$$

(105, 4) = 1100

1051-2511

7-10-1968

THE UNIVERSITY OF CHICAGO

$$C \setminus C = \emptyset$$

INVESTING

1751-1756 = 24700

01-HY-0-0644V.01

ALCOHOL CONSUMPTION

1985-1986

IV\TBA=TBVA

17

NOTES ON CONTRIBUTORS

(05.8) 31100

SYNOPSIS 18798-03

678121) ET9H=50;

מלך ישראל

$$Y \setminus \{Y\} = Y \setminus \{Y\}$$

CPA=ALV5

$$5Y \setminus X = 214$$
$$57 \text{ V} \cdot \text{A} = 302 \text{ J/s}$$

SY \set X = T2WJA

$$5Y \wedge 5X = 30Y \wedge X$$

STAY-Y-RESTAY

00-09801-00

(101) 99-500

2000-2001-2002

$$= Y \setminus \{5\} = 0 \neq \emptyset$$
$$E(X) = 34.92$$

C CHROMATOGRAPH ... (CONT'D)

```
WATER=Y4/Y3
WRITE(6,206)
WRITE(6,203)CO,CO2,BUTEN,CRACK,ALCO,ALDE,OXYGE,WATER
```

```
C      MOLE PRODUCT PER MOLE WATER
C
```

```
CO=RPTBT(4)/Y4
CO2=RPTBT(16)/Y4
BUTEN=Y1/Y4
DEHYD=Y2/Y4
CRACK=X1/Y4
ALCO=X3/Y4
ALDE=X4/Y4
ALKET=X5/Y4
OXYGE=X2/Y4
WATER=Y4/Y4
```

```
C      MOLE PRODUCT PER MOLE ETHYLENE
C
```

```
CO=RPTBT(4)/Y5
CO2=RPTBT(16)/Y5
BUTEN=Y1/Y5
DEHYD=Y2/Y5
CRACK=X1/Y5
ALCO=X3/Y5
ALDE=X4/Y5
ALKET=X5/Y5
OXYGE=X2/Y5
WATER=Y4/Y5
WRITE(6,208)
WRITE(6,203)CO,CO2,BUTEN,CRACK,ALCO,ALDE,OXYGE,WATER
WRITE(6,93)
```

```
500 CONTINUE
```

```
75 CONTINUE
```

```
CALL EXIT
```

```
END
```


RUN NO = 60

REACTOR ENTRANCE CONDITIONS

AIR = 1.68 LB/HR

BUTANE = 9.90 LB/HR

TEMPERATURE = 685.00 DEG F

PRESSURE = 53.60 LB/SQ IN

OXYGEN = 5.3497 NITROGEN = 20.1251 BUTANE = 74.5251 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 3.7030 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 13.9306

DENSITY OF GAS MIXTURE = 0.2210 LB/CU FT

GAS VELOCITY = 6.83 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.41 SEC

REYNOLDS NUMBER = 6358

RUN NO = 60 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	4.393529	0.222142	5.085697	17.492111
3	19.777946	1.000000	22.893814	78.742614
4	0.057071	0.002885	0.066062	0.227220
5	0.019322	0.000976	0.022366	0.076928
6	0.017625	0.000891	0.020401	0.070171
7	0.000000	0.000000	0.000000	0.000000
8	0.015184	0.000767	0.017576	0.060455
9	0.753493	0.038097	0.872200	2.999909
10	0.202902	0.010259	0.234868	0.807824
11	0.033678	0.001702	0.038984	0.134085
12	0.026014	0.001315	0.030112	0.103570
13	72.988403	3.690393	84.487182	290.591186
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.142664	0.007213	0.165140	0.567996
17	0.659517	0.033346	0.763419	2.625760
18	0.264578	0.013377	0.306260	1.053374
19	0.084625	0.004278	0.097957	0.336920
20	0.097405	0.004924	0.112751	0.387805
21	0.000000	0.000000	0.000000	0.000000
22	0.404339	0.020443	0.468039	1.609808
23	0.000000	0.000000	0.000000	0.000000
24	0.028200	0.001425	0.032642	0.112273
25	0.033605	0.001699	0.038899	0.133792
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
TOTALS	099.999999	100.000015	5.056138	

CARBON BALANCE 15.021898 LB AT/MOLN2. 101.41 PERCENT
HYDROGEN BALANCE 37.503631 LB AT/MOLN2. 101.27 PERCENT
OXYGEN BALANCE 0.541093 LB AT/MOLN2. 101.77 PERCENT

PERCENT O2 REACT 16.4319 PERCENT C4 REACT 0.3429

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2272	0.5679	0.2376	0.1373	0.3369	1.5534	3.6339	2.6257
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.9560	2.3899	1.0000	0.5780	1.4176	6.5365	15.2908	11.0485
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	2.4997	1.0459	0.6046	1.4827	6.8367	15.9931	11.5559
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.2380	8.0944	3.3868	1.9578	4.8014	22.1380	51.7873	37.4193

RUN NO = 60 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	4.245702	0.213955	4.125055	3.401256
3	19.843860	1.000000	19.279968	15.897029
4	0.212200	0.010693	0.206170	0.169995
5	0.036646	0.001846	0.035604	0.029357
6	0.025004	0.001260	0.024294	0.020031
7	0.000000	0.000000	0.000000	0.000000
8	0.029757	0.001499	0.028912	0.023839
9	0.842347	0.042448	0.818411	0.674809
10	0.188586	0.009503	0.183227	0.151077
11	0.123838	0.006240	0.120319	0.099207
12	0.180045	0.009073	0.174929	0.144235
13	72.235382	3.640188	70.182708	57.868171
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.198074	0.009981	0.192446	0.158678
17	0.614352	0.030959	0.596894	0.492161
18	0.360341	0.018158	0.350102	0.288671
19	0.270962	0.013654	0.263262	0.217069
20	0.089848	0.004527	0.087294	0.071977
21	0.043085	0.002171	0.041861	0.034516
22	0.390205	0.019663	0.379116	0.312595
23	0.000000	0.000000	0.000000	0.000000
24	0.029757	0.001499	0.028912	0.023839
25	0.040172	0.002024	0.039031	0.032182
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999984	100.000091	5.039344
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CARBON BALANCE	14.912012 LB AT/MOLN2.	100.67 PERCENT
HYDROGEN BALANCE	37.182304 LB AT/MOLN2.	100.40 PERCENT
OXYGEN BALANCE	0.551227 LB AT/MOLN2.	103.68 PERCENT

PERCENT O2 REACT	19.5119	PERCENT C4 REACT	1.6987
------------------	---------	------------------	--------

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1699	0.1586	0.2434	0.0531	0.2515	0.3844	0.9808	0.4921
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.6982	0.6518	1.0000	0.2185	1.0334	1.5793	4.0290	2.0216
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.9334	1.4320	0.3129	1.4799	2.2617	5.7698	2.8951
	MOLE	PRODUCT	PER MOLE	ETHENE			
8.4864	7.9214	12.1530	2.6556	12.5595	19.1942	48.9656	24.5694

RUN NO = 60 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.141659	0.007061	0.028775	0.018580
2	0.409908	0.020432	0.083265	0.053763
3	20.061649	1.000000	4.075140	2.631281
4	1.927261	0.096066	0.391486	0.252779
5	0.465459	0.023201	0.094549	0.061049
6	0.495489	0.024698	0.100649	0.064988
7	0.145908	0.007273	0.029638	0.019137
8	0.214827	0.010708	0.043638	0.028176
9	2.130676	0.106206	0.432806	0.279458
10	0.168916	0.008419	0.034312	0.022155
11	1.305461	0.065072	0.265179	0.171223
12	0.366641	0.018275	0.074476	0.048088
13	66.665863	3.323050	13.541894	8.743877
14	0.034748	0.001732	0.007058	0.004557
15	0.019819	0.000987	0.004025	0.002599
16	0.341587	0.017026	0.069386	0.044802
17	1.206030	0.060116	0.244982	0.158182
18	0.161538	0.008052	0.032813	0.021187
19	2.289994	0.114147	0.465168	0.300355
20	0.432166	0.021541	0.087786	0.056682
21	0.144930	0.007224	0.029439	0.019009
22	0.325910	0.016245	0.066202	0.042746
23	0.010999	0.000548	0.002234	0.001442
24	0.199152	0.009927	0.040454	0.026120
25	0.105573	0.005262	0.021445	0.013846
26	0.010360	0.000516	0.002104	0.001358
27	0.017845	0.000889	0.003625	0.002340
28	0.008511	0.000424	0.001729	0.001116
29	0.168864	0.008417	0.034301	0.022148
30	0.022410	0.001117	0.004552	0.002939

TOTALS	99.999923	099.999999	4.984634
--------	-----------	------------	----------

CARBON BALANCE	14.529146 LB AT/MOLN2.	98.08 PERCENT
HYDROGEN BALANCE	35.979316 LB AT/MOLN2.	97.16 PERCENT
OXYGEN BALANCE	0.425415 LB AT/MOLN2.	80.01 PERCENT

PERCENT O2 REACT	92.3135	PERCENT C4 REACT	10.2628
------------------	---------	------------------	---------

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2527	0.0448	0.2193	0.1269	0.3428	0.1063	0.5112	0.1581
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.1525	0.2042	1.0000	0.5788	1.5633	0.4848	2.3313	0.7212
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1772	0.8676	0.5021	1.3564	0.4206	2.0226	0.6257
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.8896	0.6893	3.3746	1.9533	5.2758	1.6361	7.8674	2.4340

RUN NO = 60 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.226197	0.011307	0.044903	0.027204
2	0.279954	0.013995	0.055574	0.033669
3	20.003654	1.000000	3.970971	2.405771
4	2.467779	0.123366	0.489884	0.296791
5	0.895498	0.044766	0.177767	0.107698
6	0.769117	0.038448	0.152679	0.092499
7	0.307392	0.015366	0.061021	0.036969
8	0.226652	0.011330	0.044993	0.027258
9	2.364611	0.118208	0.469404	0.284383
10	0.129199	0.006458	0.025647	0.015538
11	0.569943	0.028491	0.113140	0.068545
12	0.624766	0.031232	0.124023	0.075138
13	65.760528	3.287425	13.054271	7.908795
14	0.094914	0.004744	0.018841	0.011415
15	0.066852	0.003342	0.013271	0.008040
16	0.811726	0.040578	0.161137	0.097623
17	1.495604	0.074766	0.296895	0.179871
18	0.418364	0.020914	0.083050	0.050315
19	1.277353	0.063856	0.253570	0.153622
20	0.307709	0.015382	0.061084	0.037007
21	0.149565	0.007476	0.029690	0.017987
22	0.285472	0.014270	0.056669	0.034332
23	0.015115	0.000755	0.003000	0.001817
24	0.140824	0.007039	0.027955	0.016936
25	0.053079	0.002653	0.010537	0.006383
26	0.025628	0.001281	0.005087	0.003082
27	0.021128	0.001056	0.004194	0.002541
28	0.029476	0.001473	0.005851	0.003545
29	0.169748	0.008485	0.033697	0.020415
30	0.012318	0.000615	0.002445	0.001481
TOTALS	100.000015	099.999999	4.999088	

CARBON BALANCE 14.398527 LB AT/MOLN2. 97.20 PERCENT
HYDROGEN BALANCE 35.552436 LB AT/MOLN2. 96.00 PERCENT
OXYGEN BALANCE 0.452543 LB AT/MOLN2. 85.12 PERCENT

PERCENT O2 REACT 94.7351 PERCENT C4 REACT 11.2248

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2967	0.0976	0.1436	0.1991	0.1951	0.1067	0.3494	0.1798
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
2.0655	0.6794	1.0000	1.3858	1.3579	0.7432	2.4322	1.2518
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.3289	0.4841	0.6709	0.6573	0.3598	1.1774	0.6060
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.2085	1.0553	1.5533	2.1527	2.1092	1.1546	3.7780	1.9445

RUN NO = 61

REACTOR ENTRANCE CONDITIONS

AIR = 2.02 LB/HR BUTANE = 9.50 LB/HR

TEMPERATURE = 695.00 DEG F

PRESSURE = 53.70 LB/SQ IN

OXYGEN = 6.2973 NITROGEN = 23.6900 BUTANE = 70.0126 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.9553 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 11.1177

DENSITY OF GAS MIXTURE = 0.2138 LB/CU FT

GAS VELOCITY = 7.02 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.37 SEC

REYNOLDS NUMBER = 6088

RUN NO = 61 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.429907	0.232142	6.892628	14.317525
3	23.390373	1.000000	29.691326	61.675506
4	0.029565	0.001264	0.037530	0.077958
5	0.000000	0.000000	0.000000	0.000000
6	0.008554	0.000365	0.010858	0.022556
7	0.004910	0.000209	0.006233	0.012948
8	0.008347	0.000356	0.010596	0.022011
9	0.997943	0.042664	1.266772	2.631368
10	0.205517	0.008786	0.260879	0.541905
11	0.046349	0.001981	0.058834	0.122212
12	0.044045	0.001883	0.055910	0.116137
13	68.747787	2.939148	87.267211	181.273468
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.121740	0.005204	0.154535	0.321005
17	0.100983	0.004317	0.128186	0.266271
18	0.237484	0.010153	0.301458	0.626197
19	0.111901	0.004784	0.142045	0.295060
20	0.061248	0.002618	0.077747	0.161499
21	0.014772	0.000631	0.018752	0.038952
22	0.418164	0.017877	0.530810	1.102612
23	0.000000	0.000000	0.000000	0.000000
24	0.008674	0.000370	0.011010	0.022871
25	0.011869	0.000507	0.015067	0.031297
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	099.999999	100.000045	4.275264
--------	------------	------------	----------

CARBON BALANCE	12.003705 LB AT/MOLN2.	101.54 PERCENT
HYDROGEN BALANCE	29.910942 LB AT/MOLN2.	101.20 PERCENT
OXYGEN BALANCE	0.517219 LB AT/MOLN2.	97.28 PERCENT

PERCENT O2 REACT	12.6700	PERCENT C4 REACT	0.5486
------------------	---------	------------------	--------

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE PRODUCT	PER MOLE	N-BUTANE				
0.0779	0.3210	0.2383	0.0349	0.3340	0.8105	2.2784	0.2662
	MOLE PRODUCT	PER MOLE	N-BUTENES				
0.3270	1.3467	1.0000	0.1466	1.4013	3.4007	9.5594	1.1171
	MOLE PRODUCT	PER MOLE	CO				
1.0000	4.1176	3.0574	0.4484	4.2845	10.3974	29.2270	3.4155
	MOLE PRODUCT	PER MOLE	ETHENE				
3.4561	14.2312	10.5668	1.5498	14.8079	35.9352	101.0133	11.8047

RUN NO = 61 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.342900	0.015092	0.059797	0.041731
2	0.304917	0.013421	0.053173	0.037109
3	22.719348	1.000000	3.961939	2.764998
4	2.687829	0.118305	0.468720	0.327115
5	1.214770	0.053468	0.211839	0.147840
6	1.478911	0.065094	0.257901	0.179987
7	0.422261	0.018585	0.073636	0.051390
8	0.148640	0.006542	0.025920	0.018089
9	1.590097	0.069988	0.277290	0.193518
10	0.105422	0.004640	0.018384	0.012830
11	1.310266	0.057671	0.228492	0.159462
12	0.674069	0.029669	0.117548	0.082035
13	58.927146	2.593698	10.276077	7.171573
14	0.000000	0.000000	0.000000	0.000000
15	0.076276	0.003357	0.013301	0.009282
16	0.461047	0.020293	0.080400	0.056110
17	3.674382	0.161729	0.640761	0.447181
18	0.336667	0.014818	0.058710	0.040973
19	2.048395	0.090160	0.357211	0.249294
20	0.384697	0.016932	0.067085	0.046818
21	0.086387	0.003802	0.015064	0.010513
22	0.367920	0.016194	0.064160	0.044776
23	0.074029	0.003258	0.012909	0.009009
24	0.142382	0.006267	0.024829	0.017328
25	0.093565	0.004118	0.016316	0.011387
26	0.021443	0.000943	0.003739	0.002609
27	0.020146	0.000886	0.003513	0.002451
28	0.033295	0.001465	0.005806	0.004052
29	0.232569	0.010236	0.040556	0.028304
30	0.020382	0.000897	0.003554	0.002480

TOTALS	99.999954	100.000030	4.401533
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CARBON BALANCE	11.628322 LB AT/MOLN2.	98.36 PERCENT
HYDROGEN BALANCE	28.906322 LB AT/MOLN2.	97.80 PERCENT
OXYGEN BALANCE	0.517444 LB AT/MOLN2.	97.32 PERCENT

PERCENT O2 REACT	94.9511	PERCENT C4 REACT	12.2375
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3271	0.0561	0.2414	0.2590	0.2907	0.1075	0.4699	0.4471
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.3545	0.2323	1.0000	1.0726	1.2038	0.4454	1.9461	1.8516
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1715	0.7382	0.7919	0.8887	0.3288	1.4368	1.3670
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.8174	0.3117	1.3417	1.4392	1.6152	0.5976	2.6112	2.4845

RUN NO = 61 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.290236	0.012949	0.051272	0.031836
2	0.297002	0.013251	0.052467	0.032578
3	22.412090	1.000000	3.959286	2.458413
4	2.799656	0.124917	0.494583	0.307098
5	1.362700	0.060802	0.240732	0.149476
6	1.238020	0.055238	0.218706	0.135800
7	0.475003	0.021194	0.083913	0.052103
8	0.217859	0.009720	0.038486	0.023897
9	3.050521	0.136110	0.538900	0.334615
10	0.130753	0.005834	0.023098	0.014342
11	1.329207	0.059307	0.234815	0.145802
12	0.995022	0.044396	0.175779	0.109145
13	57.119361	2.548596	10.090620	6.265502
14	0.000000	0.000000	0.000000	0.000000
15	0.094790	0.004229	0.016745	0.010397
16	0.853443	0.038079	0.150768	0.093615
17	3.784926	0.168878	0.668639	0.415173
18	0.287751	0.012839	0.050833	0.031563
19	1.865853	0.083252	0.329618	0.204668
20	0.362083	0.016155	0.063965	0.039717
21	0.168906	0.007536	0.029838	0.018527
22	0.319808	0.014269	0.056496	0.035080
23	0.034578	0.001542	0.006108	0.003792
24	0.119924	0.005350	0.021185	0.013154
25	0.080919	0.003610	0.014295	0.008876
26	0.026755	0.001193	0.004726	0.002934
27	0.020550	0.000916	0.003630	0.002254
28	0.048357	0.002157	0.008542	0.005304
29	0.194145	0.008662	0.034297	0.021296
30	0.019895	0.000887	0.003514	0.002182
TOTALS	99.999969	99.999984	4.461873	

CARBON BALANCE 11.729370 LB AT/MOLN2. 99.22 PERCENT
HYDROGEN BALANCE 29.001487 LB AT/MOLN2. 98.13 PERCENT
OXYGEN BALANCE 0.554834 LB AT/MOLN2. 104.36 PERCENT

PERCENT O2 REACT 95.0147 PERCENT C4 REACT 13.7636

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3070	0.0936	0.2549	0.2573	0.2474	0.0866	0.3893	0.4151
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.2045	0.3671	1.0000	1.0092	0.9704	0.3400	1.5271	1.6284
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.3048	0.8301	0.8378	0.8056	0.2822	1.2678	1.3519
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.2613	0.6893	1.8773	1.8947	1.8219	0.6383	2.8671	3.0572

RUN NO = 62

REACTOR ENTRANCE CONDITIONS

AIR = 2.60 LB/HR BUTANE = 9.60 LB/HR

TEMPERATURE = 695.00 DEG F

PRESSURE = 53.70 LB/SQ IN

OXYGEN = 7.4126 NITROGEN = 27.8855 BUTANE = 64.7017 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.3202 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 8.7285

DENSITY OF GAS MIXTURE = 0.2070 LB/CU FT

GAS VELOCITY = 7.68 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.25 SEC

REYNOLDS NUMBER = 6223

RUN NO = 62 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.918601	0.221237	4.962115	5.955798
3	26.752258	1.000000	22.428909	26.920387
4	0.299170	0.011182	0.250822	0.301050
5	0.040817	0.001525	0.034221	0.041074
6	0.019715	0.000736	0.016529	0.019839
7	0.004123	0.000154	0.003457	0.004149
8	0.018926	0.000707	0.015867	0.019045
9	2.586965	0.096700	2.168893	2.603223
10	0.184649	0.006902	0.154808	0.185809
11	0.156108	0.005835	0.130880	0.157089
12	0.019684	0.000735	0.016503	0.019808
13	61.078392	2.283112	51.207702	61.462249
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	1.774366	0.066325	1.487616	1.785517
17	0.176376	0.006592	0.147872	0.177485
18	0.402461	0.015044	0.337421	0.404990
19	0.088349	0.003302	0.074072	0.088905
20	0.068041	0.002543	0.057045	0.068468
21	0.010826	0.000404	0.009076	0.010894
22	0.341729	0.012773	0.286503	0.343877
23	0.000000	0.000000	0.000000	0.000000
24	0.026286	0.000982	0.022038	0.026452
25	0.032201	0.001203	0.026997	0.032403
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999984	99.999954	3.738000	

CARBON BALANCE 9.615722 LB AT/MOLN2. 103.60 PERCENT
HYDROGEN BALANCE 23.681831 LB AT/MOLN2. 102.06 PERCENT
OXYGEN BALANCE 0.629156 LB AT/MOLN2. 118.34 PERCENT

PERCENT O2 REACT 16.7725 PERCENT C4 REACT 1.6009

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3010	1.7855	0.1768	0.0642	0.0997	0.4999	0.9759	0.1774
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.7018	10.0934	1.0000	0.3633	0.5641	2.8259	5.5172	1.0033
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	5.9309	0.5876	0.2134	0.3315	1.6605	3.2419	0.5895
	MOLE	PRODUCT	PER MOLE	ETHENE			
15.1746	90.0000	8.9166	3.2395	5.0304	25.1983	49.1954	8.9462

RUN NO = 62 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.500148	0.200303	3.057165	2.584755
3	27.459079	1.000000	15.262672	12.904201
4	0.456546	0.016626	0.253763	0.214550
5	0.044149	0.001607	0.024539	0.020747
6	0.123902	0.004512	0.068869	0.058227
7	0.024307	0.000885	0.013511	0.011423
8	0.041489	0.001510	0.023061	0.019497
9	1.761894	0.064164	0.979319	0.827989
10	0.156685	0.005706	0.087091	0.073633
11	0.174254	0.006345	0.096856	0.081889
12	0.225349	0.008206	0.125256	0.105901
13	61.584236	2.242764	34.230575	28.941078
14	0.025976	0.000946	0.014438	0.012207
15	0.000000	0.000000	0.000000	0.000000
16	0.480655	0.017504	0.267164	0.225880
17	0.807087	0.029392	0.448606	0.379285
18	0.137898	0.005021	0.076648	0.064804
19	0.308253	0.011225	0.171337	0.144861
20	0.127580	0.004646	0.070913	0.059955
21	0.052523	0.001912	0.029194	0.024683
22	0.294048	0.010708	0.163441	0.138185
23	0.000000	0.000000	0.000000	0.000000
24	0.055371	0.002016	0.030777	0.026021
25	0.053000	0.001930	0.029459	0.024907
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.097062	0.003534	0.053950	0.045613
30	0.008643	0.000314	0.004804	0.004062
TOTALS	99.999984	100.000045	3.641783	

CARBON	BALANCE	9.378070	LB AT/MOLN2.	101.04	PERCENT
HYDROGEN	BALANCE	23.287170	LB AT/MOLN2.	100.36	PERCENT
OXYGEN	BALANCE	0.522945	LB AT/MOLN2.	98.36	PERCENT

PERCENT O2 REACT	24.6477	PERCENT C4 REACT	3.3398
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2145	0.2258	0.1877	0.0516	0.2151	0.1507	0.5330	0.3792
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.1424	1.2028	1.0000	0.2751	1.1457	0.8029	2.8387	2.0197
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	1.0528	0.8752	0.2408	1.0028	0.7027	2.4846	1.7678
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.6847	3.8793	3.2251	0.8873	3.6951	2.5895	9.1554	6.5139

RUN NO = 62 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.417555	0.015330	0.064913	0.051651
2	0.807447	0.029646	0.125526	0.099880
3	27.236026	1.000000	4.234122	3.369086
4	2.663660	0.097799	0.414093	0.329493
5	1.260069	0.046264	0.195890	0.155870
6	1.247298	0.045795	0.193905	0.154290
7	0.378621	0.013901	0.058860	0.046835
8	0.193332	0.007098	0.030055	0.023915
9	1.578735	0.057964	0.245430	0.195288
10	0.131572	0.004830	0.020454	0.016275
11	0.520240	0.019101	0.080876	0.064353
12	1.009798	0.037075	0.156983	0.124911
13	55.110519	2.023442	8.567501	6.817151
14	0.026758	0.000982	0.004159	0.003309
15	0.021455	0.000787	0.003335	0.002654
16	0.461883	0.016958	0.071804	0.057134
17	3.720885	0.136616	0.578450	0.460272
18	0.216666	0.007955	0.033683	0.026801
19	1.578055	0.057939	0.245324	0.195204
20	0.599680	0.022017	0.093226	0.074180
21	0.106178	0.003898	0.016506	0.013134
22	0.285468	0.010481	0.044379	0.035312
23	0.023165	0.000850	0.003601	0.002865
24	0.121835	0.004473	0.018940	0.015070
25	0.062258	0.002285	0.009678	0.007701
26	0.020142	0.000739	0.003131	0.002491
27	0.026465	0.000971	0.004114	0.003273
28	0.006853	0.000251	0.001065	0.000847
29	0.141234	0.005185	0.021956	0.017470
30	0.026344	0.000967	0.004095	0.003258
TOTALS	99.999954	100.000045	3.671608	

CARBON BALANCE	9.016687 LB AT/MOLN2.	97.15 PERCENT
HYDROGEN BALANCE	22.439113 LB AT/MOLN2.	96.70 PERCENT
OXYGEN BALANCE	0.445642 LB AT/MOLN2.	83.82 PERCENT

PERCENT O2 REACT	88.8473	PERCENT C4 REACT	12.7923
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3294	0.0571	0.1892	0.2782	0.2283	0.1193	0.3976	0.4602
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.7409	0.3018	1.0000	1.4702	1.2062	0.6304	2.1008	2.4318
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1734	0.5744	0.8445	0.6928	0.3621	1.2067	1.3969
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.1355	0.3703	1.2266	1.8035	1.4796	0.7733	2.5770	2.9831

RUN NO = 62 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.445837	0.016676	0.066187	0.046648
2	0.370628	0.013863	0.055021	0.038779
3	26.734516	1.000000	3.968893	2.797252
4	3.324902	0.124367	0.493600	0.347887
5	1.987010	0.074323	0.294983	0.207902
6	1.446426	0.054103	0.214730	0.151340
7	0.567226	0.021216	0.084207	0.059349
8	0.202701	0.007582	0.030092	0.021208
9	2.567250	0.096027	0.381123	0.268613
10	0.127131	0.004755	0.018873	0.013301
11	0.766694	0.028678	0.113820	0.080219
12	0.705782	0.026399	0.104777	0.073846
13	52.473564	1.962764	7.790001	5.490348
14	0.028552	0.001068	0.004238	0.002987
15	0.018734	0.000700	0.002781	0.001960
16	0.407629	0.015247	0.060514	0.042650
17	4.620081	0.172813	0.685877	0.483402
18	0.335081	0.012533	0.049744	0.035059
19	1.661945	0.062164	0.246725	0.173890
20	0.446314	0.016694	0.066258	0.046698
21	0.111828	0.004182	0.016601	0.011700
22	0.164753	0.006162	0.024458	0.017238
23	0.033393	0.001249	0.004957	0.003493
24	0.116568	0.004360	0.017305	0.012196
25	0.064431	0.002410	0.009565	0.006741
26	0.017513	0.000655	0.002599	0.001832
27	0.027410	0.001025	0.004069	0.002867
28	0.023207	0.000868	0.003445	0.002428
29	0.175981	0.006582	0.026125	0.018413
30	0.027124	0.001014	0.004026	0.002838
TOTALS	99.999984	100.000045	3.740485	

CARBON BALANCE	8.969221 LB AT/MOLN2.	96.64 PERCENT
HYDROGEN BALANCE	22.332065 LB AT/MOLN2.	96.24 PERCENT
OXYGEN BALANCE	0.475304 LB AT/MOLN2.	89.40 PERCENT

PERCENT O2 REACT	94.7847	PERCENT C4 REACT	15.4074
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3478	0.0426	0.1540	0.3351	0.2058	0.0968	0.3353	0.4834
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
2.2580	0.2768	1.0000	2.1750	1.3360	0.6284	2.1769	3.1376
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1225	0.4428	0.9632	0.5916	0.2783	0.9641	1.3895
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.2987	0.2818	1.0180	2.2142	1.3600	0.6397	2.2161	3.1941

RUN NO = 62 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.699618	0.025449	0.101932	0.069420
2	0.443973	0.016150	0.064685	0.044053
3	27.490211	1.000000	4.005247	2.727754
4	3.178936	0.115638	0.463162	0.315434
5	1.745298	0.063488	0.254285	0.173179
6	1.298747	0.047244	0.189223	0.128870
7	0.514927	0.018731	0.075023	0.051094
8	0.221266	0.008048	0.032237	0.021955
9	1.014454	0.036902	0.147803	0.100660
10	0.145583	0.005295	0.021211	0.014445
11	0.319212	0.011611	0.046508	0.031674
12	1.335610	0.048584	0.194594	0.132527
13	53.706428	1.953656	7.824874	5.329094
14	0.032864	0.001195	0.004788	0.003261
15	0.024192	0.000880	0.003524	0.002400
16	0.308836	0.011234	0.044996	0.030644
17	4.116934	0.149760	0.599825	0.408508
18	0.324986	0.011821	0.047349	0.032247
19	1.786697	0.064993	0.260316	0.177287
20	0.444624	0.016173	0.064780	0.044118
21	0.054961	0.001999	0.008007	0.005453
22	0.282752	0.010285	0.041196	0.028056
23	0.023972	0.000872	0.003492	0.002378
24	0.117807	0.004285	0.017164	0.011689
25	0.065162	0.002370	0.009493	0.006465
26	0.019462	0.000707	0.002835	0.001931
27	0.057244	0.002082	0.008340	0.005680
28	0.020870	0.000759	0.003040	0.002070
29	0.179416	0.006526	0.026140	0.017802
30	0.025151	0.000914	0.003664	0.002495

TOTALS	99.999969	100.000015	3.637661
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CARBON BALANCE	8.745096 LB AT/MOLN2.	94.22 PERCENT
HYDROGEN BALANCE	21.839576 LB AT/MOLN2.	94.12 PERCENT
OXYGEN BALANCE	0.443961 LB AT/MOLN2.	83.50 PERCENT

PERCENT O2 REACT	93.9244	PERCENT C4 REACT	15.8000
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3154	0.0306	0.1642	0.3156	0.2024	0.0937	0.3376	0.4085
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.9210	0.1866	1.0000	1.9223	1.2330	0.5708	2.0564	2.4878
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.0971	0.5205	1.0006	0.6418	0.2971	1.0705	1.2950
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.4476	0.2377	1.2741	2.4493	1.5711	0.7273	2.6203	3.1699

RUN NO = 63

REACTOR ENTRANCE CONDITIONS

AIR = 3.20 LB/HR

BUTANE = 9.40 LB/HR

TEMPERATURE = 702.00 DEG F

PRESSURE = 53.60 LB/SQ IN

OXYGEN = 8.5425 NITROGEN = 32.1361 BUTANE = 59.3213 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 1.8459 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 6.9442

DENSITY OF GAS MIXTURE = 0.1986 LB/CU FT

GAS VELOCITY = 8.26 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.16 SEC

REYNOLDS NUMBER = 6167

RUN NO = 63 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	7.657487	0.241292	9.836380	17.529582
3	31.735332	1.000000	40.765434	72.648773
4	0.081563	0.002570	0.104771	0.186715
5	0.047136	0.001485	0.060549	0.107905
6	0.022835	0.000719	0.029333	0.052275
7	0.008318	0.000262	0.010685	0.019042
8	0.004079	0.000128	0.005239	0.009337
9	1.153166	0.036336	1.481292	2.639836
10	0.157146	0.004951	0.201861	0.359740
11	0.046847	0.001476	0.060177	0.107243
12	0.054015	0.001702	0.069385	0.123652
13	58.144531	1.832170	74.689208	133.104919
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.070594	0.002224	0.090681	0.161605
17	0.155665	0.004905	0.199958	0.356349
18	0.148297	0.004672	0.190495	0.339484
19	0.076758	0.002418	0.098599	0.175715
20	0.053797	0.001695	0.069105	0.123153
21	0.000000	0.000000	0.000000	0.000000
22	0.361843	0.011401	0.464803	0.828334
23	0.000000	0.000000	0.000000	0.000000
24	0.020681	0.000651	0.026565	0.047343
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999984	099.999999	3.151062
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CARBON BALANCE	7.514079 LB AT/MOLN2.	101.76 PERCENT
HYDROGEN BALANCE	18.711200 LB AT/MOLN2.	101.36 PERCENT
OXYGEN BALANCE	0.515348 LB AT/MOLN2.	96.93 PERCENT

PERCENT O2 REACT	9.2281	PERCENT C4 REACT	0.7456
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1867	0.1616	0.2308	0.1362	0.1757	0.5099	1.5140	0.3563
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.8086	0.6999	1.0000	0.5902	0.7610	2.2087	6.5571	1.5433
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.8655	1.2366	0.7299	0.9410	2.7313	8.1087	1.9085
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.5717	3.0914	4.4169	2.6070	3.3613	9.7556	28.9626	6.8167

RUN NO = 63 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.030907	0.001000	0.009732	0.007530
2	5.035277	0.163012	1.585565	1.226855
3	30.888900	1.000000	9.726654	7.526143
4	1.024332	0.033161	0.322553	0.249580
5	0.570366	0.018465	0.179603	0.138970
6	0.950611	0.030775	0.299339	0.231618
7	0.132073	0.004275	0.041588	0.032180
8	0.046799	0.001515	0.014736	0.011402
9	1.502008	0.048626	0.472969	0.365967
10	0.151369	0.004900	0.047664	0.036881
11	0.410570	0.013291	0.129285	0.100036
12	1.262007	0.040856	0.397395	0.307490
13	52.914688	1.713064	16.662387	12.892768
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.382507	0.012383	0.120448	0.093198
17	2.169321	0.070229	0.683100	0.528559
18	0.204170	0.006609	0.064291	0.049746
19	1.179424	0.038182	0.371390	0.287369
20	0.492821	0.015954	0.155185	0.120077
21	0.064737	0.002095	0.020385	0.015773
22	0.284624	0.009214	0.089625	0.069349
23	0.022738	0.000736	0.007160	0.005540
24	0.053777	0.001740	0.016934	0.013102
25	0.059616	0.001930	0.018772	0.014525
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.018055	0.000584	0.005685	0.004399
29	0.148452	0.004806	0.046746	0.036170
30	0.000000	0.000000	0.000000	0.000000

TOTALS	099.999999	100.000061	3.237409
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CARBON	BALANCE	7.507674	LB AT/MOLN2.	101.67	PERCENT
HYDROGEN	BALANCE	18.641902	LB AT/MOLN2.	100.98	PERCENT
OXYGEN	BALANCE	0.536037	LB AT/MOLN2.	100.82	PERCENT

PERCENT O2 REACT	38.6762	PERCENT C4 REACT	7.1979
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2495	0.0931	0.4075	0.1900	0.3393	0.1829	0.6160	0.5285
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.6124	0.2286	1.0000	0.4664	0.8326	0.4488	1.5116	1.2969
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.3734	1.6328	0.7616	1.3595	0.7329	2.4683	2.1177
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.0775	0.4023	1.7594	0.8206	1.4649	0.7897	2.6597	2.2820

RUN NO = 63 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.409390	0.013505	0.053660	0.038114
2	0.428792	0.014145	0.056203	0.039920
3	30.313938	1.000000	3.973336	2.822217
4	2.998391	0.098911	0.393007	0.279149
5	2.216689	0.073124	0.290547	0.206373
6	2.498659	0.082426	0.327506	0.232624
7	0.700159	0.023096	0.091771	0.065184
8	0.117671	0.003881	0.015423	0.010955
9	2.287084	0.075446	0.299774	0.212926
10	0.101054	0.003333	0.013245	0.009408
11	1.076277	0.035504	0.141070	0.100201
12	1.286836	0.042450	0.168669	0.119804
13	45.216384	1.491603	5.926642	4.209630
14	0.073986	0.002440	0.009697	0.006888
15	0.050362	0.001661	0.006601	0.004688
16	0.601949	0.019857	0.078899	0.056041
17	6.752976	0.222768	0.885132	0.628699
18	0.136290	0.004495	0.017863	0.012688
19	1.329945	0.043872	0.174319	0.123817
20	0.504077	0.016628	0.066070	0.046929
21	0.171196	0.005647	0.022439	0.015938
22	0.262960	0.008674	0.034466	0.024481
23	0.038985	0.001286	0.005109	0.003629
24	0.060240	0.001987	0.007895	0.005608
25	0.051108	0.001685	0.006698	0.004758
26	0.041797	0.001378	0.005478	0.003891
27	0.035997	0.001187	0.004718	0.003351
28	0.021633	0.000713	0.002835	0.002014
29	0.201306	0.006640	0.026385	0.018741
30	0.014057	0.000463	0.001842	0.001308
TOTALS	99.999954	100.000030	3.298814	

CARBON	BALANCE	7.117500	LB AT/MOLN2.	96.39	PERCENT
HYDROGEN	BALANCE	17.784534	LB AT/MOLN2.	96.34	PERCENT
OXYGEN	BALANCE	0.484346	LB AT/MOLN2.	91.10	PERCENT

PERCENT O2 REACT	94.6787	PERCENT C4 REACT	19.1952
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2791	0.0560	0.2200	0.3206	0.1623	0.0685	0.2671	0.6286
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.2688	0.2547	1.0000	1.4573	0.7381	0.3117	1.2143	2.8576
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2007	0.7881	1.1485	0.5817	0.2456	0.9570	2.2521
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.2000	0.2409	0.9457	1.3783	0.6980	0.2948	1.1484	2.7026

RUN NO = 63 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.820772	0.027179	0.107865	0.074891
2	0.418099	0.013845	0.054946	0.038149
3	30.198028	1.000000	3.968608	2.755437
4	3.688765	0.122152	0.484775	0.336583
5	2.366218	0.078356	0.310967	0.215907
6	2.715235	0.089914	0.356834	0.247753
7	0.734919	0.024336	0.096582	0.067058
8	0.148252	0.004909	0.019483	0.013527
9	2.518332	0.083393	0.330957	0.229786
10	0.132450	0.004386	0.017406	0.012085
11	0.672847	0.022281	0.088425	0.061394
12	0.891458	0.029520	0.117155	0.081341
13	44.784164	1.483016	5.885510	4.086357
14	0.041831	0.001385	0.005497	0.003816
15	0.038535	0.001276	0.005064	0.003516
16	0.385989	0.012781	0.050726	0.035219
17	6.867948	0.227430	0.902582	0.626670
18	0.165227	0.005471	0.021714	0.015076
19	1.172875	0.038839	0.154138	0.107019
20	0.462955	0.015330	0.060841	0.042242
21	0.102779	0.003403	0.013507	0.009378
22	0.235195	0.007788	0.030909	0.021460
23	0.025258	0.000836	0.003319	0.002304
24	0.077663	0.002571	0.010206	0.007086
25	0.069877	0.002313	0.009183	0.006376
26	0.033238	0.001100	0.004368	0.003032
27	0.023147	0.000766	0.003042	0.002112
28	0.033048	0.001094	0.004343	0.003015
29	0.159669	0.005287	0.020983	0.014569
30	0.015399	0.000509	0.002023	0.001405

TOTALS	99.999954	100.000030	3.311476
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CARBON BALANCE	7.026005 LB AT/MOLN2.	95.15 PERCENT
HYDROGEN BALANCE	17.585548 LB AT/MOLN2.	95.26 PERCENT
OXYGEN BALANCE	0.488151 LB AT/MOLN2.	91.81 PERCENT

PERCENT O2 REACT	94.7915	PERCENT C4 REACT	19.6604
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3365	0.0352	0.1427	0.3713	0.1339	0.0665	0.2350	0.6266
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
2.3580	0.2467	1.0000	2.6018	0.9387	0.4660	1.6469	4.3904
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1046	0.4240	1.1033	0.3981	0.1976	0.6984	1.8618
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.3585	0.1421	0.5761	1.4990	0.5408	0.2684	0.9488	2.5294

DATE OF DEPOSIT 10/10/50

DATE	DESCRIPTION	AMOUNT	BALANCE
10/10/50	DEPOSIT	100.00	100.00
10/11/50	WITHDRAWAL	25.00	75.00
10/12/50	DEPOSIT	50.00	125.00
10/13/50	WITHDRAWAL	10.00	115.00
10/14/50	DEPOSIT	75.00	190.00
10/15/50	WITHDRAWAL	30.00	160.00
10/16/50	DEPOSIT	15.00	175.00
10/17/50	WITHDRAWAL	40.00	135.00
10/18/50	DEPOSIT	60.00	195.00
10/19/50	WITHDRAWAL	20.00	175.00
10/20/50	DEPOSIT	80.00	255.00
10/21/50	WITHDRAWAL	15.00	240.00
10/22/50	DEPOSIT	35.00	275.00
10/23/50	WITHDRAWAL	55.00	220.00
10/24/50	DEPOSIT	45.00	265.00
10/25/50	WITHDRAWAL	65.00	200.00
10/26/50	DEPOSIT	25.00	225.00
10/27/50	WITHDRAWAL	75.00	150.00
10/28/50	DEPOSIT	55.00	205.00
10/29/50	WITHDRAWAL	35.00	170.00
10/30/50	DEPOSIT	10.00	180.00
10/31/50	WITHDRAWAL	45.00	135.00
11/01/50	DEPOSIT	65.00	200.00
11/02/50	WITHDRAWAL	25.00	175.00
11/03/50	DEPOSIT	85.00	260.00
11/04/50	WITHDRAWAL	15.00	245.00
11/05/50	DEPOSIT	35.00	280.00
11/06/50	WITHDRAWAL	55.00	225.00
11/07/50	DEPOSIT	45.00	270.00
11/08/50	WITHDRAWAL	65.00	205.00
11/09/50	DEPOSIT	25.00	230.00
11/10/50	WITHDRAWAL	75.00	155.00
11/11/50	DEPOSIT	55.00	210.00
11/12/50	WITHDRAWAL	35.00	175.00
11/13/50	DEPOSIT	10.00	185.00
11/14/50	WITHDRAWAL	45.00	140.00
11/15/50	DEPOSIT	65.00	205.00
11/16/50	WITHDRAWAL	25.00	180.00
11/17/50	DEPOSIT	85.00	265.00
11/18/50	WITHDRAWAL	15.00	250.00
11/19/50	DEPOSIT	35.00	285.00
11/20/50	WITHDRAWAL	55.00	230.00
11/21/50	DEPOSIT	45.00	275.00
11/22/50	WITHDRAWAL	65.00	210.00
11/23/50	DEPOSIT	25.00	235.00
11/24/50	WITHDRAWAL	75.00	160.00
11/25/50	DEPOSIT	55.00	215.00
11/26/50	WITHDRAWAL	35.00	180.00
11/27/50	DEPOSIT	10.00	190.00
11/28/50	WITHDRAWAL	45.00	145.00
11/29/50	DEPOSIT	65.00	210.00
11/30/50	WITHDRAWAL	25.00	185.00
11/31/50	DEPOSIT	85.00	270.00
12/01/50	WITHDRAWAL	15.00	255.00
12/02/50	DEPOSIT	35.00	290.00
12/03/50	WITHDRAWAL	55.00	235.00
12/04/50	DEPOSIT	45.00	280.00
12/05/50	WITHDRAWAL	65.00	215.00
12/06/50	DEPOSIT	25.00	240.00
12/07/50	WITHDRAWAL	75.00	165.00
12/08/50	DEPOSIT	55.00	220.00
12/09/50	WITHDRAWAL	35.00	185.00
12/10/50	DEPOSIT	10.00	195.00
12/11/50	WITHDRAWAL	45.00	150.00
12/12/50	DEPOSIT	65.00	215.00
12/13/50	WITHDRAWAL	25.00	190.00
12/14/50	DEPOSIT	85.00	275.00
12/15/50	WITHDRAWAL	15.00	260.00
12/16/50	DEPOSIT	35.00	295.00
12/17/50	WITHDRAWAL	55.00	240.00
12/18/50	DEPOSIT	45.00	285.00
12/19/50	WITHDRAWAL	65.00	220.00
12/20/50	DEPOSIT	25.00	245.00
12/21/50	WITHDRAWAL	75.00	170.00
12/22/50	DEPOSIT	55.00	225.00
12/23/50	WITHDRAWAL	35.00	190.00
12/24/50	DEPOSIT	10.00	200.00
12/25/50	WITHDRAWAL	45.00	155.00
12/26/50	DEPOSIT	65.00	220.00
12/27/50	WITHDRAWAL	25.00	195.00
12/28/50	DEPOSIT	85.00	280.00
12/29/50	WITHDRAWAL	15.00	265.00
12/30/50	DEPOSIT	35.00	300.00
12/31/50	WITHDRAWAL	55.00	245.00

DATE	DESCRIPTION	AMOUNT	BALANCE
12/31/50	DEPOSIT	100.00	345.00
1/01/51	WITHDRAWAL	25.00	320.00
1/02/51	DEPOSIT	50.00	370.00
1/03/51	WITHDRAWAL	10.00	360.00
1/04/51	DEPOSIT	75.00	435.00
1/05/51	WITHDRAWAL	30.00	405.00
1/06/51	DEPOSIT	15.00	420.00
1/07/51	WITHDRAWAL	40.00	380.00
1/08/51	DEPOSIT	60.00	440.00
1/09/51	WITHDRAWAL	20.00	420.00
1/10/51	DEPOSIT	80.00	500.00
1/11/51	WITHDRAWAL	15.00	485.00
1/12/51	DEPOSIT	35.00	520.00
1/13/51	WITHDRAWAL	55.00	465.00
1/14/51	DEPOSIT	45.00	510.00
1/15/51	WITHDRAWAL	65.00	445.00
1/16/51	DEPOSIT	25.00	470.00
1/17/51	WITHDRAWAL	75.00	395.00
1/18/51	DEPOSIT	55.00	450.00
1/19/51	WITHDRAWAL	35.00	415.00
1/20/51	DEPOSIT	10.00	425.00
1/21/51	WITHDRAWAL	45.00	380.00
1/22/51	DEPOSIT	65.00	445.00
1/23/51	WITHDRAWAL	25.00	420.00
1/24/51	DEPOSIT	85.00	505.00
1/25/51	WITHDRAWAL	15.00	490.00
1/26/51	DEPOSIT	35.00	525.00
1/27/51	WITHDRAWAL	55.00	470.00
1/28/51	DEPOSIT	45.00	515.00
1/29/51	WITHDRAWAL	65.00	450.00
1/30/51	DEPOSIT	25.00	475.00
1/31/51	WITHDRAWAL	75.00	400.00
2/01/51	DEPOSIT	55.00	455.00
2/02/51	WITHDRAWAL	35.00	420.00
2/03/51	DEPOSIT	10.00	430.00
2/04/51	WITHDRAWAL	45.00	385.00
2/05/51	DEPOSIT	65.00	450.00
2/06/51	WITHDRAWAL	25.00	425.00
2/07/51	DEPOSIT	85.00	510.00
2/08/51	WITHDRAWAL	15.00	495.00
2/09/51	DEPOSIT	35.00	530.00
2/10/51	WITHDRAWAL	55.00	475.00
2/11/51	DEPOSIT	45.00	520.00
2/12/51	WITHDRAWAL	65.00	455.00
2/13/51	DEPOSIT	25.00	480.00
2/14/51	WITHDRAWAL	75.00	405.00
2/15/51	DEPOSIT	55.00	460.00
2/16/51	WITHDRAWAL	35.00	425.00
2/17/51	DEPOSIT	10.00	435.00
2/18/51	WITHDRAWAL	45.00	390.00
2/19/51	DEPOSIT	65.00	455.00
2/20/51	WITHDRAWAL	25.00	430.00
2/21/51	DEPOSIT	85.00	515.00
2/22/51	WITHDRAWAL	15.00	500.00
2/23/51	DEPOSIT	35.00	535.00
2/24/51	WITHDRAWAL	55.00	480.00
2/25/51	DEPOSIT	45.00	525.00
2/26/51	WITHDRAWAL	65.00	460.00
2/27/51	DEPOSIT	25.00	485.00
2/28/51	WITHDRAWAL	75.00	410.00
2/29/51	DEPOSIT	55.00	465.00
2/30/51	WITHDRAWAL	35.00	430.00
3/01/51	DEPOSIT	10.00	440.00
3/02/51	WITHDRAWAL	45.00	395.00
3/03/51	DEPOSIT	65.00	460.00
3/04/51	WITHDRAWAL	25.00	435.00
3/05/51	DEPOSIT	85.00	520.00
3/06/51	WITHDRAWAL	15.00	505.00
3/07/51	DEPOSIT	35.00	540.00
3/08/51	WITHDRAWAL	55.00	485.00
3/09/51	DEPOSIT	45.00	530.00
3/10/51	WITHDRAWAL	65.00	465.00
3/11/51	DEPOSIT	25.00	490.00
3/12/51	WITHDRAWAL	75.00	415.00
3/13/51	DEPOSIT	55.00	470.00
3/14/51	WITHDRAWAL	35.00	435.00
3/15/51	DEPOSIT	10.00	445.00
3/16/51	WITHDRAWAL	45.00	400.00
3/17/51	DEPOSIT	65.00	465.00
3/18/51	WITHDRAWAL	25.00	440.00
3/19/51	DEPOSIT	85.00	525.00
3/20/51	WITHDRAWAL	15.00	510.00
3/21/51	DEPOSIT	35.00	545.00
3/22/51	WITHDRAWAL	55.00	490.00
3/23/51	DEPOSIT	45.00	535.00
3/24/51	WITHDRAWAL	65.00	470.00
3/25/51	DEPOSIT	25.00	495.00
3/26/51	WITHDRAWAL	75.00	420.00
3/27/51	DEPOSIT	55.00	475.00
3/28/51	WITHDRAWAL	35.00	440.00
3/29/51	DEPOSIT	10.00	450.00
3/30/51	WITHDRAWAL	45.00	405.00
3/31/51	DEPOSIT	65.00	470.00
4/01/51	WITHDRAWAL	25.00	445.00

DATE	DESCRIPTION	AMOUNT	BALANCE
4/02/51	DEPOSIT	85.00	530.00
4/03/51	WITHDRAWAL	15.00	515.00
4/04/51	DEPOSIT	35.00	550.00
4/05/51	WITHDRAWAL	55.00	495.00
4/06/51	DEPOSIT	45.00	540.00
4/07/51	WITHDRAWAL	65.00	475.00
4/08/51	DEPOSIT	25.00	500.00
4/09/51	WITHDRAWAL	75.00	425.00
4/10/51	DEPOSIT	55.00	480.00
4/11/51	WITHDRAWAL	35.00	445.00
4/12/51	DEPOSIT	10.00	455.00
4/13/51	WITHDRAWAL	45.00	410.00
4/14/51	DEPOSIT	65.00	475.00
4/15/51	WITHDRAWAL	25.00	450.00
4/16/51	DEPOSIT	85.00	535.00
4/17/51	WITHDRAWAL	15.00	520.00
4/18/51	DEPOSIT	35.00	555.00
4/19/51	WITHDRAWAL	55.00	500.00
4/20/51	DEPOSIT	45.00	545.00
4/21/51	WITHDRAWAL	65.00	480.00
4/22/51	DEPOSIT	25.00	505.00
4/23/51	WITHDRAWAL	75.00	430.00
4/24/51	DEPOSIT	55.00	485.00
4/25/51	WITHDRAWAL	35.00	450.00
4/26/51	DEPOSIT	10.00	460.00
4/27/51	WITHDRAWAL	45.00	415.00
4/28/51	DEPOSIT	65.00	480.00
4/29/51	WITHDRAWAL	25.00	455.00
4/30/51	DEPOSIT	85.00	540.00
5/01/51	WITHDRAWAL	15.00	525.00
5/02/51	DEPOSIT	35.00	560.00
5/03/51	WITHDRAWAL	55.00	505.00
5/04/51	DEPOSIT	45.00	550.00
5/05/51	WITHDRAWAL	65.00	485.00
5/06/51	DEPOSIT	25.00	510.00
5/07/51	WITHDRAWAL	75.00	435.00
5/08/51	DEPOSIT	55.00	490.00
5/09/51	WITHDRAWAL	35.00	455.00
5/10/51	DEPOSIT	10.00	465.00
5/11/51	WITHDRAWAL	45.00	420.00
5/12/51	DEPOSIT	65.00	485.00
5/13/51	WITHDRAWAL	25.00	460.00
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6/01/51	DEPOSIT	45.00	560.00
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6/28/51	WITHDRAWAL	55.00	525.00
6/29/51	DEPOSIT	45.00	570.00
6/30/51	WITHDRAWAL	65.00	505.00
7/01/51	DEPOSIT	25.00	530.00
7/02/51	WITHDRAWAL	75.00	455.00
7/03/51	DEPOSIT	55.00	510.00
7/04/51	WITHDRAWAL	35.00	475.00
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11/01/51	WITHDRAWAL	55.00	570.00
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11/03/51	WITHDRAWAL	65.00	550.00
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12/23/51	WITHDRAWAL	25.00	540.00
12/24/51	DEPOSIT	85.00	625.00
12/25/51	WITHDRAWAL	15.00	610.00
12/26/51	DEPOSIT	35.00	645.00
12/27/51	WITHDRAWAL	55.00	590.00
12/28/51	DEPOSIT	45.00	635.00
12/29/51	WITHDRAWAL	65.00	570.00
12/30/51	DEPOSIT	25.00	595.00
12/31/51	WITHDRAWAL	75.00	520.00

RUN NO = 63 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.666795	0.021975	0.087149	0.060515
2	0.414724	0.013667	0.054203	0.037638
3	30.343265	1.000000	3.965815	2.753847
4	3.810564	0.125581	0.498034	0.345833
5	2.446556	0.080629	0.319760	0.222040
6	2.598112	0.085624	0.339568	0.235795
7	0.786565	0.025922	0.102802	0.071385
8	0.167878	0.005532	0.021941	0.015236
9	1.682586	0.055451	0.219911	0.152705
10	0.111528	0.003675	0.014576	0.010121
11	0.886227	0.029206	0.115828	0.080430
12	1.148003	0.037833	0.150042	0.104188
13	44.993194	1.482806	5.880536	4.083421
14	0.060375	0.001989	0.007890	0.005479
15	0.049091	0.001617	0.006416	0.004455
16	0.394046	0.012986	0.051501	0.035762
17	6.537186	0.215441	0.854399	0.593291
18	0.277729	0.009152	0.036298	0.025205
19	1.274978	0.042018	0.166637	0.115712
20	0.476697	0.015710	0.062303	0.043263
21	0.089746	0.002957	0.011729	0.008145
22	0.268981	0.008864	0.035155	0.024411
23	0.029727	0.000979	0.003885	0.002697
24	0.084243	0.002776	0.011010	0.007645
25	0.079112	0.002607	0.010339	0.007179
26	0.035286	0.001162	0.004611	0.003202
27	0.022697	0.000748	0.002966	0.002059
28	0.040110	0.001321	0.005242	0.003640
29	0.202589	0.006676	0.026478	0.018386
30	0.021600	0.000711	0.002823	0.001960
TOTALS	99.999954	100.000030	3.295624	

CARBON BALANCE 7.024767 LB AT/MOLN2. 95.13 PERCENT
HYDROGEN BALANCE 17.559226 LB AT/MOLN2. 95.12 PERCENT
OXYGEN BALANCE 0.490019 LB AT/MOLN2. 92.17 PERCENT

PERCENT O2 REACT 94.8583 PERCENT C4 REACT 19.6717

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3458	0.0357	0.1846	0.3691	0.1454	0.0781	0.2635	0.5932
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.8732	0.1937	1.0000	1.9996	0.7878	0.4234	1.4273	3.2135
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1034	0.5338	1.0675	0.4205	0.2260	0.7619	1.7155
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.4666	0.1516	0.7829	1.5656	0.6168	0.3315	1.1175	2.5161

RUN NO = 64

REACTOR ENTRANCE CONDITIONS

AIR = 2.50 LB/HR BUTANE = 8.20 LB/HR

TEMPERATURE = 692.00 DEG F

PRESSURE = 53.58 LB/SQ IN

OXYGEN = 7.9898 NITROGEN = 30.0572 BUTANE = 61.9528 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.0611 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 7.7538

DENSITY OF GAS MIXTURE = 0.2036 LB/CU FT

GAS VELOCITY = 6.84 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.41 SEC

REYNOLDS NUMBER = 5370

RUN NO = 64 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	6.970619	0.234989	7.621179	33.067695
3	29.663585	1.000000	32.432060	140.720153
4	0.021427	0.000722	0.023427	0.101649
5	0.004032	0.000135	0.004408	0.019127
6	0.029030	0.000978	0.031740	0.137718
7	0.002504	0.000084	0.002738	0.011881
8	0.004466	0.000150	0.004883	0.021187
9	0.967696	0.032622	1.058010	4.590621
10	0.144446	0.004869	0.157927	0.685234
11	0.007480	0.000252	0.008178	0.035485
12	0.027343	0.000921	0.029894	0.129711
13	60.930694	2.054057	66.617294	289.047119
14	0.010948	0.000369	0.011970	0.051939
15	0.000000	0.000000	0.000000	0.000000
16	0.636260	0.021449	0.695641	3.018333
17	0.028656	0.000966	0.031330	0.135941
18	0.098604	0.003324	0.107807	0.467768
19	0.012299	0.000414	0.013446	0.058345
20	0.049133	0.001656	0.053719	0.233083
21	0.000000	0.000000	0.000000	0.000000
22	0.285185	0.009614	0.311801	1.352883
23	0.000000	0.000000	0.000000	0.000000
24	0.060674	0.002045	0.066337	0.287831
25	0.044997	0.001516	0.049197	0.213463
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999984	99.999984	3.371137	

CARBON	BALANCE	8.401590 LB AT/MOLN2.	101.90 PERCENT
HYDROGEN	BALANCE	20.880924 LB AT/MOLN2.	101.30 PERCENT
OXYGEN	BALANCE	0.533136 LB AT/MOLN2.	100.28 PERCENT

PERCENT O2 REACT	11.5993	PERCENT C4 REACT	0.3447
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1016	3.0183	0.1651	0.0521	0.0583	0.9886	2.6133	0.1359
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.6153	18.2710	1.0000	0.3159	0.3531	5.9848	15.8197	0.8229
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	29.6935	1.6251	0.5134	0.5739	9.7264	25.7096	1.3373
	MOLE	PRODUCT	PER MOLE	ETHENE			
0.7380	21.9166	1.1995	0.3790	0.4236	7.1790	18.9762	0.9870

RUN NO = 64 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	6.202250	0.209448	3.715347	2.714990
3	29.612247	1.000000	17.738689	12.962547
4	0.221516	0.007480	0.132695	0.096967
5	0.156373	0.005280	0.093672	0.068451
6	0.063684	0.002150	0.038148	0.027877
7	0.015429	0.000521	0.009242	0.006754
8	0.027751	0.000937	0.016623	0.012147
9	2.517343	0.085010	1.507969	1.101948
10	0.150590	0.005085	0.090208	0.065919
11	0.155970	0.005267	0.093431	0.068275
12	0.095724	0.003232	0.057341	0.041902
13	58.751220	1.984017	35.193870	25.717922
14	0.062549	0.002112	0.037469	0.027380
15	0.000000	0.000000	0.000000	0.000000
16	1.172799	0.039605	0.702544	0.513384
17	0.122429	0.004134	0.073339	0.053592
18	0.031309	0.001057	0.018755	0.013705
19	0.115934	0.003915	0.069448	0.050749
20	0.092113	0.003110	0.055178	0.040321
21	0.016359	0.000552	0.009800	0.007161
22	0.309779	0.010461	0.185567	0.135603
23	0.000000	0.000000	0.000000	0.000000
24	0.070367	0.002376	0.042152	0.030803
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.036373	0.001228	0.021789	0.015922
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999969	099.999999	3.376981
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CARBON BALANCE	8.360897 LB AT/MOLN2.	101.40 PERCENT
HYDROGEN BALANCE	20.641960 LB AT/MOLN2.	100.14 PERCENT
OXYGEN BALANCE	0.532423 LB AT/MOLN2.	100.14 PERCENT

PERCENT O2 REACT	21.2073	PERCENT C4 REACT	3.7428
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.0969	0.5133	0.1101	0.0873	0.0579	0.0848	0.2942	0.0535
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.8800	4.6596	1.0000	0.7928	0.5256	0.7699	2.6708	0.4864
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	5.2944	1.1362	0.9008	0.5972	0.8748	3.0347	0.5526
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.4783	18.4158	3.9522	3.1334	2.0773	3.0429	10.5557	1.9224

RUN NO = 64 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.573815	0.019986	0.080352	0.065248
2	0.490452	0.017083	0.068678	0.055769
3	28.709751	1.000000	4.020269	3.264598
4	2.471805	0.086096	0.346130	0.281070
5	1.527088	0.053190	0.213840	0.173645
6	1.882644	0.065575	0.263629	0.214076
7	0.420999	0.014664	0.058953	0.047872
8	0.073687	0.002566	0.010318	0.008379
9	3.047624	0.106152	0.426763	0.346546
10	0.096536	0.003362	0.013518	0.010977
11	0.992995	0.034587	0.139050	0.112913
12	0.973959	0.033924	0.136384	0.110749
13	50.381210	1.754846	7.054955	5.728870
14	0.037751	0.001314	0.005286	0.004292
15	0.030897	0.001076	0.004326	0.003513
16	0.901998	0.031417	0.126308	0.102566
17	4.566679	0.159063	0.639478	0.519279
18	0.233911	0.008147	0.032754	0.026598
19	1.488973	0.051863	0.208503	0.169311
20	0.332118	0.011568	0.046507	0.037765
21	0.105674	0.003680	0.014797	0.012016
22	0.217728	0.007583	0.030488	0.024758
23	0.042113	0.001466	0.005897	0.004788
24	0.061566	0.002144	0.008621	0.007000
25	0.047189	0.001643	0.006607	0.005365
26	0.021707	0.000756	0.003039	0.002468
27	0.020133	0.000701	0.002819	0.002289
28	0.037451	0.001304	0.005244	0.004258
29	0.191276	0.006662	0.026784	0.021750
30	0.020474	0.000713	0.002867	0.002328
TOTALS	99.999969	100.000030	3.483139	

CARBON BALANCE	8.138820 LB AT/MOLN2.	98.71 PERCENT
HYDROGEN BALANCE	20.190696 LB AT/MOLN2.	97.95 PERCENT
OXYGEN BALANCE	0.440397 LB AT/MOLN2.	82.83 PERCENT

PERCENT O2 REACT	93.5734	PERCENT C4 REACT	14.8613
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2810	0.1025	0.2236	0.2951	0.2055	0.0736	0.3206	0.5192
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.2566	0.4585	1.0000	1.3195	0.9190	0.3293	1.4338	2.3217
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.3649	0.7957	1.0500	0.7313	0.2620	1.1409	1.8475
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.3129	0.4791	1.0447	1.3786	0.9601	0.3440	1.4980	2.4256

RUN NO = 64 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.860754	0.029921	0.118408	0.084431
2	0.377567	0.013125	0.051939	0.037035
3	28.767009	1.000000	3.957296	2.821745
4	2.955873	0.102752	0.406620	0.289940
5	2.227372	0.077428	0.306405	0.218482
6	2.161430	0.075135	0.297334	0.212013
7	0.687290	0.023891	0.094546	0.067416
8	0.111819	0.003887	0.015382	0.010968
9	1.349076	0.046896	0.185584	0.132330
10	0.109867	0.003819	0.015113	0.010776
11	0.733587	0.025500	0.100914	0.071957
12	0.886041	0.030800	0.121887	0.086911
13	49.098739	1.706772	6.754204	4.816077
14	0.053925	0.001874	0.007418	0.005289
15	0.048008	0.001668	0.006604	0.004709
16	0.572718	0.019908	0.078785	0.056177
17	6.390933	0.222161	0.879160	0.626884
18	0.244768	0.008508	0.033671	0.024009
19	1.013994	0.035248	0.139488	0.099462
20	0.470619	0.016359	0.064740	0.046162
21	0.109912	0.003820	0.015119	0.010781
22	0.265836	0.009241	0.036569	0.026075
23	0.043620	0.001516	0.006000	0.004278
24	0.104554	0.003634	0.014382	0.010255
25	0.056197	0.001953	0.007730	0.005512
26	0.032100	0.001115	0.004415	0.003148
27	0.040608	0.001411	0.005586	0.003983
28	0.028133	0.000977	0.003870	0.002759
29	0.181558	0.006311	0.024975	0.017808
30	0.016276	0.000565	0.002239	0.001596

TOTALS	099.999999	100.000045	3.476204
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CARBON	BALANCE	7.800337 LB AT/MOLN2.	94.61 PERCENT
HYDROGEN	BALANCE	19.592727 LB AT/MOLN2.	95.05 PERCENT
OXYGEN	BALANCE	0.481647 LB AT/MOLN2.	90.59 PERCENT

PERCENT O2 REACT	95.0624	PERCENT C4 REACT	17.1937
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2899	0.0561	0.1588	0.3812	0.1312	0.0844	0.2558	0.6268
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.8250	0.3536	1.0000	2.4000	0.8258	0.5313	1.6103	3.9459
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1937	0.5479	1.3150	0.4525	0.2911	0.8823	2.1621
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.3675	0.2649	0.7493	1.7984	0.6188	0.3981	1.2066	2.9568

RUN NO = 64 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.867718	0.031067	0.122950	0.086365
2	0.367024	0.013140	0.052004	0.036530
3	27.930305	1.000000	3.957543	2.779954
4	3.194267	0.114365	0.452606	0.317931
5	2.328342	0.083362	0.329911	0.231744
6	2.261506	0.080969	0.320440	0.225091
7	0.862370	0.030875	0.122192	0.085833
8	0.116660	0.004176	0.016529	0.011611
9	2.619298	0.093779	0.371137	0.260703
10	0.112747	0.004036	0.015975	0.011221
11	0.625527	0.022396	0.088633	0.062259
12	1.037733	0.037154	0.147040	0.103287
13	47.521881	1.701445	6.733541	4.729940
14	0.055552	0.001988	0.007871	0.005529
15	0.048552	0.001738	0.006879	0.004832
16	0.335033	0.011995	0.047472	0.033346
17	6.826504	0.244412	0.967271	0.679454
18	0.247902	0.008875	0.035126	0.024674
19	1.503299	0.053823	0.213007	0.149626
20	0.331213	0.011858	0.046930	0.032966
21	0.096240	0.003445	0.013636	0.009579
22	0.195577	0.007002	0.027712	0.019466
23	0.033438	0.001197	0.004737	0.003328
24	0.064454	0.002307	0.009132	0.006415
25	0.071016	0.002542	0.010062	0.007068
26	0.031560	0.001129	0.004471	0.003141
27	0.029982	0.001073	0.004248	0.002984
28	0.028933	0.001035	0.004099	0.002879
29	0.216701	0.007758	0.030705	0.021568
30	0.038854	0.001391	0.005505	0.003867

TOTALS	100.000030	100.000045	3.580343
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CARBON BALANCE	7.981754 LB AT/MOLN2.	96.81 PERCENT
HYDROGEN BALANCE	20.051712 LB AT/MOLN2.	97.28 PERCENT
OXYGEN BALANCE	0.512491 LB AT/MOLN2.	96.39 PERCENT

PERCENT O2 REACT	95.0565	PERCENT C4 REACT	17.4521
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3179	0.0333	0.1655	0.4155	0.1839	0.0670	0.2875	0.6794
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.9204	0.2014	1.0000	2.5101	1.1109	0.4049	1.7370	4.1042
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1048	0.5207	1.3070	0.5784	0.2108	0.9044	2.1371
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.4124	0.1481	0.7354	1.8461	0.8170	0.2978	1.2775	3.0185

RUN NO = 65

REACTOR ENTRANCE CONDITIONS

AIR = 2.95 LB/HR

BUTANE = 9.20 LB/HR

TEMPERATURE = 687.00 DEG F

PRESSURE = 53.47 LB/SQ IN

OXYGEN = 8.2410 NITROGEN = 31.0020 BUTANE = 60.7568 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 1.9597 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 7.3724

DENSITY OF GAS MIXTURE = 0.2026 LB/CU FT

GAS VELOCITY = 7.81 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.23 SEC

REYNOLDS NUMBER = 6072

RUN NO = 65 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	7.199123	0.234868	7.587571	16.622116
3	30.651729	1.000000	32.305625	70.772033
4	0.058561	0.001910	0.061721	0.135213
5	0.054990	0.001794	0.057958	0.126968
6	0.028495	0.000929	0.030032	0.065792
7	0.001882	0.000061	0.001983	0.004345
8	0.003691	0.000120	0.003890	0.008523
9	0.990311	0.032308	1.043746	2.286538
10	0.149536	0.004878	0.157604	0.345265
11	0.026498	0.000864	0.027928	0.061182
12	0.132536	0.004323	0.139687	0.306013
13	59.637145	1.945637	62.855026	137.696685
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.082486	0.002691	0.086937	0.190453
17	0.148426	0.004842	0.156435	0.342704
18	0.273058	0.008908	0.287791	0.630465
19	0.100812	0.003288	0.106252	0.232767
20	0.045209	0.001474	0.047649	0.104385
21	0.025941	0.000846	0.027341	0.059896
22	0.347589	0.011339	0.366344	0.802551
23	0.000000	0.000000	0.000000	0.000000
24	0.042068	0.001372	0.044337	0.097131
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS 099.999999 99.999969 3.262459

CARBON BALANCE 7.972114 LB AT/MOLN2. 101.69 PERCENT
HYDROGEN BALANCE 19.857952 LB AT/MOLN2. 101.32 PERCENT
OXYGEN BALANCE 0.509102 LB AT/MOLN2. 95.75 PERCENT

PERCENT O2 REACT 11.6447 PERCENT C4 REACT 0.7209

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1352	0.1904	0.3671	0.1398	0.2926	0.8319	1.9271	0.3427
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.3682	0.5186	1.0000	0.3808	0.7970	2.2657	5.2484	0.9332
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	1.4085	2.7156	1.0342	2.1644	6.1531	14.2530	2.5345
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.0551	2.8947	5.5810	2.1254	4.4482	12.6454	29.2918	5.2088

RUN NO = 65 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.869879	0.192478	2.624301	3.078124
3	30.496330	1.000000	13.634277	15.992071
4	0.311511	0.010214	0.139270	0.163354
5	0.116816	0.003830	0.052226	0.061258
6	0.122901	0.004030	0.054946	0.064448
7	0.016033	0.000525	0.007168	0.008407
8	0.010783	0.000353	0.004820	0.005654
9	1.288694	0.042257	0.576148	0.675782
10	0.134624	0.004414	0.060187	0.070596
11	0.387000	0.012690	0.173020	0.202940
12	0.351809	0.011536	0.157286	0.184486
13	57.858734	1.897236	25.867439	30.340728
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.127525	0.004181	0.057013	0.066873
17	0.576548	0.018905	0.257762	0.302337
18	0.188316	0.006175	0.084192	0.098752
19	1.453767	0.047670	0.649949	0.762345
20	0.132053	0.004330	0.059038	0.069248
21	0.022551	0.000739	0.010082	0.011825
22	0.275722	0.009041	0.123269	0.144586
23	0.000000	0.000000	0.000000	0.000000
24	0.059868	0.001963	0.026766	0.031394
25	0.053443	0.001752	0.023893	0.028025
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.024833	0.000814	0.011102	0.013022
29	0.120429	0.003948	0.053841	0.063152
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999923	100.000045	3.279085	

CARBON BALANCE 7.971753 LB AT/MOLN2. 101.69 PERCENT
HYDROGEN BALANCE 19.870773 LB AT/MOLN2. 101.39 PERCENT
OXYGEN BALANCE 0.498874 LB AT/MOLN2. 93.83 PERCENT

PERCENT O2 REACT 27.5915 PERCENT C4 REACT 3.1907

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1633	0.0668	0.3874	0.0753	0.8373	0.1993	1.2223	0.3023
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.4216	0.1726	1.0000	0.1944	2.1612	0.5146	3.1550	0.7803
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.4093	2.3716	0.4610	5.1258	1.2206	7.4828	1.8508
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.5346	1.0376	6.0114	1.1686	12.9921	3.0938	18.9663	4.6911

RUN NO = 65 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.645106	0.021176	0.083430	0.065751
2	0.365560	0.012000	0.047277	0.037259
3	30.463356	1.000000	3.939757	3.104948
4	2.088984	0.068573	0.270163	0.212917
5	1.535403	0.050401	0.198570	0.156494
6	1.618265	0.053121	0.209286	0.164940
7	0.439259	0.014419	0.056808	0.044771
8	0.130481	0.004283	0.016874	0.013299
9	1.290527	0.042363	0.166901	0.131535
10	0.111633	0.003664	0.014437	0.011378
11	0.513146	0.016844	0.066364	0.052301
12	1.295655	0.042531	0.167564	0.132058
13	49.889854	1.637700	6.452141	5.084975
14	0.034760	0.001141	0.004495	0.003542
15	0.034816	0.001142	0.004502	0.003548
16	0.422845	0.013880	0.054685	0.043098
17	5.320844	0.174663	0.688132	0.542322
18	0.146228	0.004800	0.018911	0.014904
19	2.141420	0.070294	0.276945	0.218262
20	0.546768	0.017948	0.070712	0.055728
21	0.067901	0.002228	0.008781	0.006920
22	0.307080	0.010080	0.039714	0.031298
23	0.049105	0.001611	0.006350	0.005005
24	0.119322	0.003916	0.015431	0.012161
25	0.071067	0.002332	0.009190	0.007243
26	0.041001	0.001345	0.005302	0.004179
27	0.039216	0.001287	0.005071	0.003997
28	0.039790	0.001306	0.005145	0.004055
29	0.210503	0.006910	0.027223	0.021455
30	0.020302	0.000666	0.002625	0.002069

TOTALS	99.999984	100.000061	3.282633
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CARBON BALANCE	7.427664 LB AT/MOLN2.	94.75 PERCENT
HYDROGEN BALANCE	18.671127 LB AT/MOLN2.	95.27 PERCENT
OXYGEN BALANCE	0.419728 LB AT/MOLN2.	78.94 PERCENT

PERCENT O2 REACT	95.4857	PERCENT C4 REACT	16.4339
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2129	0.0430	0.1843	0.2803	0.2508	0.0867	0.3872	0.5423
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.1548	0.2337	1.0000	1.5204	1.3604	0.4707	2.1006	2.9416
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2024	0.8658	1.3165	1.1780	0.4076	1.8189	2.5470
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.2908	0.2612	1.1177	1.6995	1.5206	0.5262	2.3480	3.2879

RUN NO = 65 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.812555	0.026985	0.106675	0.076763
2	0.386904	0.012849	0.050794	0.036551
3	30.110332	1.000000	3.952988	2.844575
4	2.466875	0.081927	0.323859	0.233049
5	2.234274	0.074202	0.293323	0.211075
6	1.776444	0.058997	0.233217	0.167823
7	0.763129	0.025344	0.100186	0.072094
8	0.125014	0.004151	0.016412	0.011810
9	0.947249	0.031459	0.124358	0.089488
10	0.127287	0.004227	0.016710	0.012025
11	0.379138	0.012591	0.049774	0.035817
12	1.163611	0.038644	0.152762	0.109928
13	48.424064	1.608220	6.357276	4.574705
14	0.053353	0.001771	0.007004	0.005040
15	0.188701	0.006266	0.024773	0.017826
16	0.464381	0.015422	0.060965	0.043870
17	6.197464	0.205825	0.813624	0.585485
18	0.140305	0.004659	0.018419	0.013254
19	1.904916	0.063264	0.250083	0.179960
20	0.437568	0.014532	0.057445	0.041337
21	0.072098	0.002394	0.009465	0.006811
22	0.291376	0.009676	0.038252	0.027526
23	0.035655	0.001184	0.004681	0.003368
24	0.111156	0.003691	0.014593	0.010501
25	0.071426	0.002372	0.009377	0.006747
26	0.019376	0.000643	0.002543	0.001830
27	0.023961	0.000795	0.003145	0.002263
28	0.046800	0.001554	0.006144	0.004421
29	0.196913	0.006539	0.025851	0.018602
30	0.027876	0.000925	0.003659	0.002633

TOTALS	99.999984	100.000015	3.321120
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CARBON BALANCE	7.327700 LB AT/MOLN2.	93.47 PERCENT
HYDROGEN BALANCE	18.522842 LB AT/MOLN2.	94.51 PERCENT
OXYGEN BALANCE	0.456532 LB AT/MOLN2.	85.87 PERCENT

PERCENT O2 REACT	95.1661	PERCENT C4 REACT	17.9381
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2330	0.0438	0.1457	0.3717	0.2072	0.0673	0.3192	0.5854
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.5990	0.3010	1.0000	2.5506	1.4216	0.4621	2.1905	4.0171
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1882	0.6253	1.5951	0.8891	0.2890	1.3699	2.5122
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.3886	0.2614	0.8684	2.2150	1.2346	0.4013	1.9023	3.4886

RUN NO = 65 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.895310	0.029480	0.115889	0.082206
2	0.347419	0.011439	0.044970	0.031899
3	30.369655	1.000000	3.931080	2.788519
4	2.460268	0.081010	0.318459	0.225900
5	2.196832	0.072336	0.284360	0.201711
6	1.828020	0.060192	0.236620	0.167847
7	0.710834	0.023406	0.092011	0.065268
8	0.150978	0.004971	0.019542	0.013862
9	0.930045	0.030624	0.120386	0.085396
10	0.057163	0.001882	0.007399	0.005248
11	0.255698	0.008419	0.033097	0.023478
12	1.506942	0.049620	0.195060	0.138366
13	48.626487	1.601153	6.294262	4.464848
14	0.032371	0.001065	0.004190	0.002972
15	0.019792	0.000651	0.002561	0.001817
16	0.346361	0.011404	0.044833	0.031802
17	5.996156	0.197439	0.776148	0.550562
18	0.211997	0.006980	0.027441	0.019465
19	1.864790	0.061403	0.241380	0.171223
20	0.344688	0.011349	0.044616	0.031649
21	0.030832	0.001015	0.003990	0.002830
22	0.305613	0.010063	0.039558	0.028061
23	0.028192	0.000928	0.003649	0.002588
24	0.091497	0.003012	0.011843	0.008401
25	0.067468	0.002221	0.008733	0.006194
26	0.028326	0.000932	0.003666	0.002600
27	0.034481	0.001135	0.004463	0.003166
28	0.034361	0.001131	0.004447	0.003155
29	0.192874	0.006350	0.024965	0.017709
30	0.034731	0.001143	0.004495	0.003189

TOTALS	99.999954	100.000030	3.292761
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CARBON	BALANCE	7.267541	LB AT/MOLN2.	92.70	PERCENT
HYDROGEN	BALANCE	18.356693	LB AT/MOLN2.	93.66	PERCENT
OXYGEN	BALANCE	0.431806	LB AT/MOLN2.	81.22	PERCENT

PERCENT O2 REACT	95.6965	PERCENT C4 REACT	18.2987
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2259	0.0318	0.1618	0.3630	0.1943	0.0626	0.3002	0.5505
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.3957	0.1965	1.0000	2.2431	1.2009	0.3872	1.8550	3.4018
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1407	0.7164	1.6071	0.8604	0.2774	1.3290	2.4371
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.3458	0.1894	0.9642	2.1629	1.1579	0.3734	1.7887	3.2801

RUN NO = 66

REACTOR ENTRANCE CONDITIONS

AIR = 2.85 LB/HR

BUTANE = 9.40 LB/HR

TEMPERATURE = 708.00 DEG F

PRESSURE = 53.40 LB/SQ IN

OXYGEN = 7.9624 NITROGEN = 29.9540 BUTANE = 62.0835 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.0726 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 7.7970

DENSITY OF GAS MIXTURE = 0.2003 LB/CU FT

GAS VELOCITY = 7.97 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.21 SEC

REYNOLDS NUMBER = 6080

RUN NO = 66 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	6.576795	0.224218	5.389362	5.733351
3	29.332046	1.000000	24.036178	25.570350
4	0.097794	0.003334	0.080137	0.085252
5	0.136555	0.004655	0.111900	0.119042
6	0.079419	0.002707	0.065080	0.069234
7	0.024160	0.000823	0.019798	0.021062
8	0.009873	0.000336	0.008090	0.008607
9	1.996633	0.068070	1.636143	1.740574
10	0.124050	0.004229	0.101653	0.108141
11	0.357504	0.012188	0.292957	0.311655
12	0.132832	0.004528	0.108849	0.115797
13	59.647338	2.033521	48.878082	51.997848
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.179830	0.006130	0.147362	0.156768
17	0.275342	0.009387	0.225629	0.240030
18	0.145173	0.004949	0.118962	0.126556
19	0.348926	0.011895	0.285928	0.304178
20	0.076268	0.002600	0.062498	0.066487
21	0.045593	0.001554	0.037361	0.039746
22	0.303899	0.010360	0.249030	0.264925
23	0.000000	0.000000	0.000000	0.000000
24	0.073162	0.002494	0.059952	0.063779
25	0.036902	0.001258	0.030239	0.032169
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	099.999999	100.000015	3.409240
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CARBON BALANCE	8.501394 LB AT/MOLN2.	102.54 PERCENT
HYDROGEN BALANCE	21.116664 LB AT/MOLN2.	101.88 PERCENT
OXYGEN BALANCE	0.508532 LB AT/MOLN2.	95.65 PERCENT

PERCENT O2 REACT	15.6510	PERCENT C4 REACT	1.8868
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.0852	0.1567	0.4274	0.1487	0.3439	0.2568	0.8978	0.2400
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.1994	0.3667	1.0000	0.3479	0.8045	0.6008	2.1004	0.5615
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	1.8388	5.0139	1.7443	4.0341	3.0124	10.5315	2.8155
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.2313	2.2643	6.1739	2.1479	4.9675	3.7094	12.9681	3.4669

RUN NO = 66 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.292503	0.010588	0.062348	0.057334
2	2.652030	0.095999	0.565295	0.519834
3	27.625328	1.000000	5.888493	5.414947
4	1.949549	0.070571	0.415557	0.382138
5	1.323973	0.047926	0.282212	0.259517
6	1.832028	0.066316	0.390507	0.359102
7	0.280251	0.010144	0.059737	0.054933
8	0.048450	0.001753	0.010327	0.009496
9	2.153348	0.077948	0.458998	0.422086
10	0.110785	0.004010	0.023614	0.021715
11	0.471870	0.017081	0.100581	0.092493
12	1.218301	0.044100	0.259687	0.238803
13	52.155380	1.887955	11.117212	10.223176
14	0.027397	0.000991	0.005839	0.005370
15	0.018168	0.000657	0.003872	0.003561
16	0.479456	0.017355	0.102198	0.093980
17	3.860398	0.139741	0.822865	0.756691
18	0.236508	0.008561	0.050413	0.046358
19	1.806731	0.065401	0.385114	0.354144
20	0.599046	0.021684	0.127690	0.117421
21	0.087453	0.003165	0.018641	0.017142
22	0.311721	0.011283	0.066445	0.061101
23	0.044717	0.001618	0.009531	0.008765
24	0.096143	0.003480	0.020493	0.018845
25	0.075703	0.002740	0.016136	0.014838
26	0.017246	0.000624	0.003676	0.003380
27	0.012858	0.000465	0.002740	0.002520
28	0.029182	0.001056	0.006220	0.005720
29	0.183618	0.006646	0.039139	0.035991
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999954	99.999984	3.619867
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CARBON BALANCE	8.553070 LB AT/MOLN2.	103.16 PERCENT
HYDROGEN BALANCE	21.290554 LB AT/MOLN2.	102.72 PERCENT
OXYGEN BALANCE	0.563752 LB AT/MOLN2.	106.03 PERCENT

PERCENT O2 REACT	63.8857	PERCENT C4 REACT	8.9101
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3821	0.0939	0.3312	0.3812	0.4106	0.1851	0.6862	0.7566
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.1534	0.2836	1.0000	1.1508	1.2395	0.5588	2.0713	2.2840
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2459	0.8669	0.9977	1.0746	0.4845	1.7957	1.9801
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.0641	0.2617	0.9225	1.0617	1.1435	0.5155	1.9109	2.1071

RUN NO = 66 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.711144	0.024922	0.098214	0.073403
2	0.344286	0.012065	0.047548	0.035536
3	28.534118	1.000000	3.940780	2.945241
4	2.603590	0.091244	0.359575	0.268738
5	2.186338	0.076621	0.301950	0.225670
6	2.040808	0.071521	0.281851	0.210648
7	0.606807	0.021266	0.083804	0.062633
8	0.121839	0.004269	0.016826	0.012576
9	2.030655	0.071165	0.280449	0.209600
10	0.128525	0.004504	0.017750	0.013266
11	0.751217	0.026327	0.103748	0.077539
12	1.105054	0.038727	0.152616	0.114061
13	49.452438	1.733098	6.829759	5.104393
14	0.033360	0.001169	0.004607	0.003443
15	0.017231	0.000603	0.002379	0.001778
16	0.362979	0.012720	0.050130	0.037466
17	5.816845	0.203855	0.803350	0.600404
18	0.308799	0.010822	0.042647	0.031873
19	1.561435	0.054721	0.215646	0.161168
20	0.472348	0.016553	0.065234	0.048754
21	0.072445	0.002538	0.010005	0.007477
22	0.261596	0.009167	0.036128	0.027001
23	0.036339	0.001273	0.005018	0.003750
24	0.059320	0.002078	0.008192	0.006122
25	0.074017	0.002593	0.010222	0.007639
26	0.024020	0.000841	0.003317	0.002479
27	0.026734	0.000936	0.003692	0.002759
28	0.041441	0.001452	0.005723	0.004277
29	0.192122	0.006733	0.026533	0.019830
30	0.022303	0.000781	0.003080	0.002302

TOTALS	99.999969	99.999984	3.504576
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CARBON BALANCE	7.995847 LB AT/MOLN2.	96.44 PERCENT
HYDROGEN BALANCE	20.056278 LB AT/MOLN2.	96.76 PERCENT
OXYGEN BALANCE	0.455170 LB AT/MOLN2.	85.61 PERCENT

PERCENT O2 REACT	95.4609	PERCENT C4 REACT	16.3816
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2687	0.0374	0.1916	0.3742	0.1909	0.0895	0.3254	0.6004
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.4025	0.1955	1.0000	1.9534	0.9966	0.4671	1.6985	3.1336
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1394	0.7129	1.3927	0.7105	0.3330	1.2109	2.2341
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.2757	0.1778	0.9095	1.7768	0.9065	0.4249	1.5449	2.8502

RUN NO = 66 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.681124	0.024399	0.096092	0.066706
2	0.332485	0.011910	0.046906	0.032562
3	27.915916	1.000000	3.938366	2.733984
4	2.836228	0.101598	0.400133	0.277770
5	2.365887	0.084750	0.333778	0.231706
6	2.295572	0.082231	0.323858	0.224820
7	0.817500	0.029284	0.115332	0.080063
8	0.174100	0.006236	0.024562	0.017050
9	1.938088	0.069425	0.273424	0.189809
10	0.127111	0.004553	0.017932	0.012448
11	0.730807	0.026178	0.103101	0.071572
12	1.170438	0.041927	0.165125	0.114628
13	47.648635	1.706862	6.722249	4.666536
14	0.045719	0.001637	0.006450	0.004477
15	0.027227	0.000975	0.003841	0.002666
16	0.570790	0.020446	0.080526	0.055901
17	7.147294	0.256029	1.008337	0.699980
18	0.223866	0.008019	0.031582	0.021924
19	1.468780	0.052614	0.207214	0.143847
20	0.580070	0.020779	0.081836	0.056809
21	0.099344	0.003558	0.014015	0.009729
22	0.282037	0.010103	0.039789	0.027621
23	0.031858	0.001141	0.004494	0.003120
24	0.102518	0.003672	0.014463	0.010040
25	0.099913	0.003579	0.014095	0.009785
26	0.020092	0.000719	0.002834	0.001967
27	0.025290	0.000905	0.003568	0.002476
28	0.040517	0.001451	0.005716	0.003968
29	0.180859	0.006478	0.025515	0.017712
30	0.020083	0.000719	0.002833	0.001966

TOTALS	100.000045	99.999984	3.582186
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CARBON BALANCE	7.984290 LB AT/MOLN2.	96.30 PERCENT
HYDROGEN BALANCE	20.082843 LB AT/MOLN2.	96.89 PERCENT
OXYGEN BALANCE	0.536084 LB AT/MOLN2.	100.83 PERCENT

PERCENT O2 REACT	95.5194	PERCENT C4 REACT	17.6474
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2777	0.0559	0.1862	0.3955	0.1732	0.0912	0.3109	0.6999
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.4917	0.3002	1.0000	2.1241	0.9304	0.4900	1.6700	3.7592
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2012	0.6703	1.4239	0.6237	0.3285	1.1195	2.5199
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.2355	0.2486	0.8282	1.7593	0.7706	0.4058	1.3831	3.1135

RUN NO = 66 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.822368	0.028506	0.112642	0.077042
2	0.367814	0.012749	0.050380	0.034457
3	28.848171	1.000000	3.951434	2.702589
4	2.177479	0.075480	0.298256	0.203993
5	2.111129	0.073180	0.289168	0.197777
6	2.311686	0.080132	0.316639	0.216566
7	0.789810	0.027378	0.108183	0.073991
8	0.167591	0.005809	0.022955	0.015700
9	0.784133	0.027181	0.107405	0.073460
10	0.103311	0.003581	0.014150	0.009678
11	1.243364	0.043100	0.170307	0.116482
12	1.201871	0.041661	0.164624	0.112595
13	49.117286	1.702613	6.727765	4.601464
14	0.023837	0.000826	0.003265	0.002233
15	0.017757	0.000615	0.002432	0.001663
16	0.405336	0.014050	0.055520	0.037973
17	6.897265	0.239088	0.944742	0.646157
18	0.331956	0.011507	0.045469	0.031098
19	1.252144	0.043404	0.171510	0.117304
20	0.471424	0.016341	0.064572	0.044164
21	0.254313	0.008815	0.034834	0.023824
22	0.011474	0.000397	0.001571	0.001074
23	0.011311	0.000392	0.001549	0.001059
24	0.022990	0.000796	0.003149	0.002153
25	0.049527	0.001716	0.006783	0.004639
26	0.017092	0.000592	0.002341	0.001601
27	0.033455	0.001159	0.004582	0.003134
28	0.028052	0.000972	0.003842	0.002628
29	0.114915	0.003983	0.015740	0.010765
30	0.011305	0.000391	0.001548	0.001059

TOTALS	99.999954	100.000030	3.466425
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CARBON BALANCE	7.791213 LB AT/MOLN2.	93.97 PERCENT
HYDROGEN BALANCE	19.681510 LB AT/MOLN2.	94.95 PERCENT
OXYGEN BALANCE	0.458642 LB AT/MOLN2.	86.26 PERCENT

PERCENT O2 REACT	95.2035	PERCENT C4 REACT	17.8524
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2039	0.0379	0.2290	0.3645	0.1534	0.0805	0.2445	0.6461
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.8904	0.1657	1.0000	1.5912	0.6700	0.3516	1.0673	2.8206
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1861	1.1229	1.7868	0.7524	0.3948	1.1986	3.1675
	MOLE	PRODUCT	PER MOLE	ETHENE			
0.9419	0.1753	1.0577	1.6831	0.7087	0.3719	1.1290	2.9836

RUN NO = 67

REACTOR ENTRANCE CONDITIONS

AIR = 2.70 LB/HR

BUTANE = 6.55 LB/HR

TEMPERATURE = 684.00 DEG F

PRESSURE = 53.59 LB/SQ IN

OXYGEN = 9.5267 NITROGEN = 35.8386 BUTANE = 54.6346 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 1.5244 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 5.7348

DENSITY OF GAS MIXTURE = 0.1957 LB/CU FT

GAS VELOCITY = 6.15 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.56 SEC

REYNOLDS NUMBER = 4446

RUN NO = 67 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	7.673542	0.216631	4.403876	5.016197
3	35.422088	1.000000	20.328876	23.155426
4	0.199976	0.005645	0.114767	0.130724
5	0.074151	0.002093	0.042555	0.048472
6	0.051544	0.001455	0.029581	0.033694
7	0.005744	0.000162	0.003297	0.003755
8	0.005008	0.000141	0.002874	0.003273
9	1.972891	0.055696	1.132250	1.289679
10	0.130058	0.003671	0.074640	0.085019
11	0.163370	0.004612	0.093758	0.106795
12	0.069045	0.001949	0.039625	0.045134
13	52.469818	1.481274	30.112632	34.299530
14	0.021826	0.000616	0.012526	0.014268
15	0.000000	0.000000	0.000000	0.000000
16	0.813178	0.022956	0.466686	0.531574
17	0.176423	0.004980	0.101249	0.115327
18	0.151545	0.004278	0.086972	0.099065
19	0.206876	0.005840	0.118727	0.135234
20	0.052086	0.001470	0.029892	0.034049
21	0.019272	0.000544	0.011060	0.012598
22	0.273838	0.007730	0.157157	0.179008
23	0.000000	0.000000	0.000000	0.000000
24	0.047773	0.001348	0.027417	0.031229
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	099.999999	99.999954	2.823096
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CARBON	BALANCE	6.203589 LB AT/MOLN2.	101.73 PERCENT
HYDROGEN	BALANCE	15.348619 LB AT/MOLN2.	100.68 PERCENT
OXYGEN	BALANCE	0.511015 LB AT/MOLN2.	96.11 PERCENT

PERCENT O2 REACT	18.5052	PERCENT C4 REACT	2.8328
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1307	0.5315	0.1519	0.0555	0.1478	0.1643	0.4911	0.1153
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.8604	3.4988	1.0000	0.3653	0.9730	1.0817	3.2329	0.7590
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	4.0663	1.1622	0.4245	1.1308	1.2571	3.7574	0.8822
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.8797	15.7763	4.5090	1.6472	4.3874	4.8774	14.5776	3.4227

RUN NO = 67 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	1.870375	0.056812	0.311195	0.300598
2	2.741068	0.083259	0.456061	0.440532
3	32.921821	1.000000	5.477568	5.291049
4	4.767739	0.144820	0.793261	0.766249
5	1.531762	0.046527	0.254856	0.246178
6	2.276088	0.069136	0.378698	0.365802
7	0.305517	0.009280	0.050832	0.049101
8	0.018727	0.000568	0.003115	0.003009
9	0.927462	0.028171	0.154312	0.149057
10	0.095899	0.002912	0.015955	0.015412
11	0.249209	0.007569	0.041463	0.040051
12	1.273913	0.038695	0.211955	0.204737
13	43.965835	1.335462	7.315083	7.065993
14	0.010723	0.000325	0.001784	0.001723
15	0.014491	0.000440	0.002411	0.002329
16	0.618791	0.018795	0.102955	0.099449
17	3.799139	0.115398	0.632104	0.610580
18	0.228242	0.006932	0.037975	0.036682
19	1.300024	0.039488	0.216299	0.208934
20	0.441048	0.013396	0.073382	0.070883
21	0.032586	0.000989	0.005421	0.005237
22	0.195483	0.005937	0.032524	0.031417
23	0.047630	0.001446	0.007924	0.007654
24	0.067940	0.002063	0.011303	0.010919
25	0.068625	0.002084	0.011417	0.011029
26	0.015466	0.000469	0.002573	0.002485
27	0.016693	0.000507	0.002777	0.002682
28	0.018689	0.000567	0.003109	0.003003
29	0.179114	0.005440	0.029801	0.028786
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999969	99.999969	3.037497
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CARBON	BALANCE	6.127145	LB AT/MOLN2.	100.48	PERCENT
HYDROGEN	BALANCE	15.155858	LB AT/MOLN2.	99.41	PERCENT
OXYGEN	BALANCE	0.543655	LB AT/MOLN2.	102.25	PERCENT

PERCENT O2 REACT	68.6784	PERCENT C4 REACT	12.3977
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.7662	0.0994	0.2447	0.5988	0.2454	0.1211	0.4197	0.6105
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
3.1302	0.4062	1.0000	2.4465	1.0026	0.4949	1.7145	2.4943
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1297	0.3194	0.7815	0.3203	0.1581	0.5477	0.7968
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.0947	0.2718	0.6691	1.6371	0.6709	0.3312	1.1473	1.6691

RUN NO = 67 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	1.006406	0.030371	0.120081	0.118483
2	0.427317	0.012895	0.050986	0.050307
3	33.136169	1.000000	3.953711	3.901108
4	3.304882	0.099736	0.394328	0.389082
5	2.839341	0.085687	0.338782	0.334274
6	1.981892	0.059810	0.236473	0.233327
7	0.710594	0.021444	0.084786	0.083657
8	0.027698	0.000835	0.003304	0.003260
9	0.882223	0.026624	0.105264	0.103863
10	0.101210	0.003054	0.012076	0.011915
11	0.384807	0.011612	0.045914	0.045303
12	1.195314	0.036072	0.142621	0.140723
13	42.020736	1.268123	5.013792	4.947085
14	0.028209	0.000851	0.003365	0.003321
15	0.019359	0.000584	0.002309	0.002279
16	0.393232	0.011867	0.046919	0.046295
17	8.421228	0.254140	1.004796	0.991427
18	0.312216	0.009422	0.037252	0.036757
19	1.468082	0.044304	0.175167	0.172836
20	0.471353	0.014224	0.056240	0.055492
21	0.056059	0.001691	0.006688	0.006599
22	0.225477	0.006804	0.026903	0.026545
23	0.056456	0.001703	0.006736	0.006646
24	0.072959	0.002201	0.008705	0.008589
25	0.111073	0.003352	0.013252	0.013076
26	0.020355	0.000614	0.002428	0.002396
27	0.012979	0.000391	0.001548	0.001528
28	0.064640	0.001950	0.007712	0.007610
29	0.219899	0.006636	0.026237	0.025888
30	0.028030	0.000845	0.003344	0.003300
TOTALS	99.999969	100.000030	3.017852	

CARBON BALANCE	5.889678 LB AT/MOLN2.	96.58 PERCENT
HYDROGEN BALANCE	14.995624 LB AT/MOLN2.	98.36 PERCENT
OXYGEN BALANCE	0.497546 LB AT/MOLN2.	93.58 PERCENT

PERCENT O2 REACT	95.1487	PERCENT C4 REACT	16.8149
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3890	0.0462	0.1860	0.5396	0.2077	0.1023	0.3672	0.9914
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
2.0915	0.2488	1.0000	2.9010	1.1166	0.5502	1.9742	5.3294
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1189	0.4781	1.3870	0.5338	0.2630	0.9439	2.5481
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.6675	0.1984	0.7972	2.3129	0.8902	0.4387	1.5740	4.2490

RUN NO = 67 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	1.653044	0.049694	0.197557	0.329111
2	0.475015	0.014280	0.056769	0.094572
3	33.264389	1.000000	3.975468	6.622746
4	3.450763	0.103737	0.412405	0.687026
5	2.698674	0.081128	0.322521	0.537290
6	1.625840	0.048876	0.194306	0.323695
7	0.668292	0.020090	0.079868	0.133053
8	0.035120	0.001055	0.004197	0.006992
9	1.011212	0.030399	0.120851	0.201326
10	0.114075	0.003429	0.013633	0.022711
11	0.579741	0.017428	0.069285	0.115423
12	1.086466	0.032661	0.129844	0.216309
13	45.687492	1.373465	5.460168	9.096113
14	0.032763	0.000984	0.003915	0.006522
15	0.013449	0.000404	0.001607	0.002677
16	0.364984	0.010972	0.043619	0.072666
17	4.586176	0.137870	0.548099	0.913081
18	0.283749	0.008530	0.033911	0.056492
19	1.330731	0.040004	0.159037	0.264940
20	0.332381	0.009992	0.039723	0.066175
21	0.035392	0.001063	0.004229	0.007046
22	0.274655	0.008256	0.032824	0.054682
23	0.020519	0.000616	0.002452	0.004085
24	0.071603	0.002152	0.008557	0.014255
25	0.058530	0.001759	0.006995	0.011653
26	0.021979	0.000660	0.002626	0.004376
27	0.013590	0.000408	0.001624	0.002705
28	0.030095	0.000904	0.003596	0.005991
29	0.160211	0.004816	0.019147	0.031897
30	0.019304	0.000580	0.002307	0.003843

TOTALS	099.999999	100.000061	3.006219
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CARBON	BALANCE	6.273664	LB AT/MOLN2.	102.88	PERCENT
HYDROGEN	BALANCE	15.748727	LB AT/MOLN2.	103.30	PERCENT
OXYGEN	BALANCE	0.371859	LB AT/MOLN2.	69.94	PERCENT

PERCENT O2 REACT	94.6280	PERCENT C4 REACT	9.9048
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.6870	0.0726	0.3317	1.0064	0.3082	0.1396	0.5281	0.9130
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
2.0710	0.2190	1.0000	3.0339	0.9292	0.4209	1.5920	2.7524
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1057	0.4828	1.4649	0.4486	0.2032	0.7687	1.3290
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.1224	0.2244	1.0248	3.1092	0.9523	0.4313	1.6316	2.8208

RUN NO = 67 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	1.167412	0.035956	0.142180	0.143773
2	0.419878	0.012932	0.051137	0.051710
3	32.467681	1.000000	3.954281	3.998578
4	3.685602	0.113516	0.448874	0.453902
5	3.147505	0.096942	0.383338	0.387633
6	2.257431	0.069528	0.274935	0.278015
7	0.655603	0.020192	0.079846	0.080741
8	0.040008	0.001232	0.004872	0.004927
9	1.385786	0.042682	0.168776	0.170667
10	0.111754	0.003442	0.013610	0.013763
11	0.554604	0.017081	0.067545	0.068302
12	1.400357	0.043130	0.170551	0.172461
13	41.375885	1.274371	5.039222	5.095673
14	0.029720	0.000915	0.003619	0.003660
15	0.024354	0.000750	0.002966	0.002999
16	0.487605	0.015018	0.059386	0.060051
17	7.633905	0.235123	0.929743	0.940158
18	0.230591	0.007102	0.028084	0.028398
19	1.639491	0.050496	0.199675	0.201912
20	0.447784	0.013791	0.054536	0.055147
21	0.037294	0.001148	0.004542	0.004593
22	0.236745	0.007291	0.028833	0.029156
23	0.017279	0.000532	0.002104	0.002128
24	0.130028	0.004004	0.015836	0.016013
25	0.074301	0.002288	0.009049	0.009150
26	0.026042	0.000802	0.003171	0.003207
27	0.029688	0.000914	0.003615	0.003656
28	0.031590	0.000972	0.003847	0.003890
29	0.232120	0.007149	0.028270	0.028586
30	0.022106	0.000680	0.002692	0.002722

TOTALS	100.000045	100.000015	3.079986
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CARBON	BALANCE	6.062321	LB AT/MOLN2.	99.41	PERCENT
HYDROGEN	BALANCE	15.326272	LB AT/MOLN2.	100.53	PERCENT
OXYGEN	BALANCE	0.501715	LB AT/MOLN2.	94.37	PERCENT

PERCENT O2 REACT	95.1350	PERCENT C4 REACT	16.4050
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.4539	0.0600	0.2407	0.6170	0.2382	0.1032	0.3885	0.9401
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.8852	0.2494	1.0000	2.5629	0.9897	0.4287	1.6138	3.9048
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1322	0.5304	1.3594	0.5250	0.2273	0.8560	2.0712
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.6326	0.2160	0.8660	2.2195	0.8571	0.3712	1.3976	3.3816

RUN NO = 68

REACTOR ENTRANCE CONDITIONS

AIR = 2.42 LB/HR BUTANE = 8.20 LB/HR

TEMPERATURE = 692.00 DEG F

PRESSURE = 53.71 LB/SQ IN

OXYGEN = 7.8295 NITROGEN = 29.4540 BUTANE = 62.7164 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.1293 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 8.0102

DENSITY OF GAS MIXTURE = 0.2051 LB/CU FT

GAS VELOCITY = 6.74 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.43 SEC

REYNOLDS NUMBER = 5357

RUN NO = 68 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	7.060018	0.241592	9.970903	21.400512
3	29.222785	1.000000	41.271507	88.580871
4	0.049888	0.001707	0.070458	0.151224
5	0.065846	0.002253	0.092995	0.199595
6	0.025196	0.000862	0.035585	0.076375
7	0.009248	0.000316	0.013061	0.028034
8	0.011163	0.000382	0.015766	0.033840
9	0.641188	0.021941	0.905553	1.943585
10	0.183626	0.006283	0.259336	0.556612
11	0.020181	0.000690	0.028502	0.061175
12	0.010828	0.000370	0.015293	0.032823
13	61.894195	2.118011	87.413513	187.615295
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.055432	0.001896	0.078286	0.168027
17	0.021847	0.000747	0.030855	0.066225
18	0.184541	0.006314	0.260629	0.559387
19	0.079098	0.002706	0.111711	0.239765
20	0.035055	0.001199	0.049509	0.106262
21	0.000000	0.000000	0.000000	0.000000
22	0.369497	0.012644	0.521843	1.120030
23	0.000000	0.000000	0.000000	0.000000
24	0.060471	0.002069	0.085403	0.183302
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	100.000015	100.000030	3.421988
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CARBON	BALANCE	8.619522	LB AT/MOLN2.	101.20	PERCENT
HYDROGEN	BALANCE	21.493236	LB AT/MOLN2.	100.94	PERCENT
OXYGEN	BALANCE	0.514369	LB AT/MOLN2.	96.75	PERCENT

PERCENT O2 REACT	9.1150	PERCENT C4 REACT	0.5301
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1512	0.1680	0.0939	0.2614	0.2397	0.8489	2.2087	0.0662
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.6087	1.7875	1.0000	2.7816	2.5507	9.0314	23.4974	0.7045
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	1.1111	0.6215	1.7290	1.5854	5.6138	14.6057	0.4379
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.9799	2.1999	1.2307	3.4234	3.1392	11.1154	28.9194	0.8670

RUN NO = 68 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.130325	0.004434	0.036614	0.027010
2	4.253040	0.144711	1.194865	0.881458
3	29.389774	1.000000	8.256877	6.091139
4	1.218770	0.041469	0.342405	0.252594
5	0.702383	0.023898	0.197330	0.145571
6	0.544775	0.018536	0.153051	0.112906
7	0.050789	0.001728	0.014268	0.010526
8	0.011385	0.000387	0.003198	0.002359
9	0.978931	0.033308	0.275024	0.202887
10	0.126504	0.004304	0.035540	0.026218
11	0.171018	0.005818	0.048046	0.035444
12	0.861983	0.029329	0.242168	0.178649
13	57.754661	1.965127	16.225822	11.969867
14	0.012158	0.000413	0.003415	0.002519
15	0.003054	0.000103	0.000858	0.000633
16	0.290889	0.009897	0.081723	0.060287
17	1.024562	0.034861	0.287844	0.212344
18	0.142697	0.004855	0.040090	0.029574
19	1.368448	0.046562	0.384457	0.283615
20	0.332496	0.011313	0.093412	0.068911
21	0.038416	0.001307	0.010792	0.007961
22	0.259388	0.008825	0.072873	0.053759
23	0.004015	0.000136	0.001128	0.000832
24	0.052421	0.001783	0.014727	0.010864
25	0.048567	0.001652	0.013644	0.010065
26	0.007092	0.000241	0.001992	0.001469
27	0.007518	0.000255	0.002112	0.001558
28	0.014159	0.000481	0.003978	0.002934
29	0.187503	0.006379	0.052677	0.038860
30	0.012385	0.000421	0.003479	0.002566

TOTALS	99.999923	99.999923	3.402543
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CARBON	BALANCE	8.374593	LB AT/MOLN2.	98.32	PERCENT
HYDROGEN	BALANCE	20.826858	LB AT/MOLN2.	97.81	PERCENT
OXYGEN	BALANCE	0.469765	LB AT/MOLN2.	88.36	PERCENT

PERCENT O2 REACT	45.5608	PERCENT C4 REACT	7.7101
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2525	0.0602	0.2140	0.1854	0.3319	0.1109	0.5129	0.2123
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.1798	0.2815	1.0000	0.8662	1.5502	0.5180	2.3960	0.9918
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2386	0.8475	0.7342	1.3139	0.4390	2.0308	0.8406
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.2371	0.5339	1.8961	1.6426	2.9396	0.9823	4.5433	1.8807

RUN NO = 68 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.734781	0.025177	0.100592	0.068240
2	0.453102	0.015525	0.062030	0.042080
3	29.183528	1.000000	3.995258	2.710327
4	2.627480	0.090032	0.359705	0.244018
5	1.924935	0.065959	0.263525	0.178772
6	1.693382	0.058025	0.231826	0.157267
7	0.358307	0.012277	0.049052	0.033276
8	0.018255	0.000625	0.002499	0.001695
9	1.004846	0.034431	0.137564	0.093321
10	0.131684	0.004512	0.018027	0.012229
11	0.438242	0.015016	0.059995	0.040700
12	0.979638	0.033568	0.134113	0.090980
13	51.372978	1.760341	7.033019	4.771100
14	0.032603	0.001117	0.004463	0.003027
15	0.027348	0.000937	0.003744	0.002539
16	0.369206	0.012651	0.050544	0.034288
17	5.155985	0.176674	0.705860	0.478845
18	0.191391	0.006558	0.026201	0.017774
19	1.918674	0.065745	0.262668	0.178190
20	0.517634	0.017737	0.070864	0.048073
21	0.059864	0.002051	0.008195	0.005559
22	0.246394	0.008442	0.033731	0.022883
23	0.045532	0.001560	0.006233	0.004228
24	0.105162	0.003603	0.014396	0.009766
25	0.058143	0.001992	0.007959	0.005399
26	0.028982	0.000993	0.003967	0.002691
27	0.017357	0.000594	0.002376	0.001612
28	0.038230	0.001310	0.005233	0.003550
29	0.230481	0.007897	0.031553	0.021405
30	0.036039	0.001234	0.004933	0.003347
TOTALS	99.999969	100.000045	3.426592	

CARBON BALANCE	7.878467 LB AT/MOLN2.	92.50 PERCENT
HYDROGEN BALANCE	19.802715 LB AT/MOLN2.	93.00 PERCENT
OXYGEN BALANCE	0.442782 LB AT/MOLN2.	83.28 PERCENT

PERCENT O2 REACT	94.1592	PERCENT C4 REACT	17.3277
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2440	0.0342	0.1316	0.2819	0.2078	0.0772	0.3244	0.4788
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.8531	0.2603	1.0000	2.1414	1.5784	0.5864	2.4641	3.6364
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1405	0.5396	1.1555	0.8517	0.3164	1.3297	1.9623
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.5516	0.2180	0.8373	1.7930	1.3216	0.4910	2.0632	3.0447

RUN NO = 68 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.427013	0.014772	0.058848	0.040805
2	0.427775	0.014798	0.058953	0.040878
3	28.906398	1.000000	3.983683	2.762290
4	2.873094	0.099393	0.395950	0.274552
5	2.319273	0.080233	0.319626	0.221629
6	1.634071	0.056529	0.225196	0.156151
7	0.555669	0.019223	0.076578	0.053099
8	0.030003	0.001037	0.004134	0.002867
9	1.410427	0.048792	0.194375	0.134780
10	0.119659	0.004139	0.016490	0.011434
11	0.444931	0.015392	0.061317	0.042517
12	1.047393	0.036233	0.144344	0.100088
13	51.085769	1.767282	7.040291	4.881748
14	0.037147	0.001285	0.005119	0.003549
15	0.017412	0.000602	0.002399	0.001663
16	0.355509	0.012298	0.048993	0.033972
17	4.924702	0.170367	0.678688	0.470603
18	0.302620	0.010468	0.041705	0.028918
19	1.805202	0.062449	0.248780	0.172504
20	0.378032	0.013077	0.052097	0.036124
21	0.084788	0.002933	0.011685	0.008102
22	0.304273	0.010526	0.041932	0.029076
23	0.023066	0.000797	0.003178	0.002204
24	0.106652	0.003689	0.014698	0.010191
25	0.076180	0.002635	0.010498	0.007279
26	0.019358	0.000669	0.002667	0.001849
27	0.021668	0.000749	0.002986	0.002070
28	0.030518	0.001055	0.004205	0.002916
29	0.203338	0.007034	0.028022	0.019430
30	0.028205	0.000975	0.003887	0.002695
TOTALS	99.999954	99.999969	3.459443	

CARBON BALANCE	7.984902 LB AT/MOLN2.	93.75 PERCENT
HYDROGEN BALANCE	20.012500 LB AT/MOLN2.	93.98 PERCENT
OXYGEN BALANCE	0.441018 LB AT/MOLN2.	82.95 PERCENT

PERCENT O2 REACT	94.4328	PERCENT C4 REACT	17.0017
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2745	0.0339	0.1426	0.3184	0.2018	0.0773	0.3233	0.4706
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.9252	0.2382	1.0000	2.2327	1.4157	0.5420	2.2675	3.3000
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1237	0.5194	1.1597	0.7353	0.2815	1.1777	1.7140
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.7582	0.2175	0.9132	2.0390	1.2928	0.4950	2.0708	3.0137

RUN NO = 68 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	1.041387	0.035832	0.144240	0.090815
2	0.505673	0.017399	0.070039	0.044097
3	29.062511	1.000000	4.025389	2.534433
4	2.767229	0.095216	0.383283	0.241319
5	2.380744	0.081918	0.329752	0.207615
6	1.761209	0.060600	0.243941	0.153588
7	0.625104	0.021508	0.086581	0.054513
8	0.020977	0.000721	0.002905	0.001829
9	0.831714	0.028618	0.115199	0.072530
10	0.141815	0.004879	0.019642	0.012367
11	0.211916	0.007291	0.029352	0.018480
12	1.390697	0.047851	0.192622	0.121277
13	50.415763	1.734735	6.982983	4.396570
14	0.034876	0.001200	0.004830	0.003041
15	0.018551	0.000638	0.002569	0.001617
16	0.369285	0.012706	0.051149	0.032204
17	5.202730	0.179018	0.720619	0.453710
18	0.136239	0.004687	0.018870	0.011880
19	1.836131	0.063178	0.254318	0.160122
20	0.428157	0.014732	0.059303	0.037338
21	0.040612	0.001397	0.005625	0.003541
22	0.305550	0.010513	0.042321	0.026645
23	0.034125	0.001174	0.004726	0.002975
24	0.085382	0.002937	0.011826	0.007445
25	0.073451	0.002527	0.010173	0.006405
26	0.023596	0.000811	0.003268	0.002057
27	0.033638	0.001157	0.004659	0.002933
28	0.019569	0.000673	0.002710	0.001706
29	0.173429	0.005967	0.024021	0.015124
30	0.028064	0.000965	0.003887	0.002447
TOTALS	99.999969	99.999954	3.440858	

CARBON BALANCE	7.810264 LB AT/MOLN2.	91.69 PERCENT
HYDROGEN BALANCE	19.669914 LB AT/MOLN2.	92.37 PERCENT
OXYGEN BALANCE	0.445172 LB AT/MOLN2.	83.73 PERCENT

PERCENT O2 REACT	93.4544	PERCENT C4 REACT	18.5302
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2413	0.0322	0.1397	0.3547	0.1808	0.0595	0.2806	0.4537
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.7266	0.2304	1.0000	2.5384	1.2939	0.4264	2.0079	3.2464
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1334	0.5791	1.4701	0.7494	0.2469	1.1628	1.8801
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.5712	0.2096	0.9099	2.3098	1.1774	0.3880	1.8271	2.9540

RUN NO = 71

REACTOR ENTRANCE CONDITIONS

AIR = 2.20 LB/HR BUTANE = 10.00 LB/HR

TEMPERATURE = 698.00 DEG F

PRESSURE = 51.40 LB/SQ IN

OXYGEN = 6.4485 NITROGEN = 24.2588 BUTANE = 69.2925 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.8563 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 10.7454

DENSITY OF GAS MIXTURE = 0.2032 LB/CU FT

GAS VELOCITY = 7.82 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.23 SEC

REYNOLDS NUMBER = 6402

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WATER TREATMENT

DATE = 10.00.1974

TEMPERATURE = 20.00 DEG C

PRESSURE = 21.00 LB/20 IN

OXYGEN = 0.4482 MILLIGRAMS PER LITER = 0.0004482 PERCENT

OXYGEN = 0.2682 MILLIGRAMS PER LITER = 0.0002682 PERCENT

RELATIVE HUMIDITY = 10.14%

DEW POINT OF THE AIR = 0.0005 PERCENT

WIND VELOCITY = 1.50 FT/SEC

RESIDUAL CHLORINE IN TREATMENT = 1.00 PERCENT

WATER TREATMENT

RUN NO = 71 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	4.466441	0.188671	2.445493	2.862056
3	23.673061	1.000000	12.961620	15.169492
4	0.504902	0.021328	0.276447	0.323536
5	0.171084	0.007226	0.093673	0.109629
6	0.222409	0.009395	0.121775	0.142518
7	0.047903	0.002023	0.026228	0.030696
8	0.023688	0.001000	0.012970	0.015179
9	0.834239	0.035240	0.456768	0.534573
10	0.220949	0.009333	0.120975	0.141582
11	0.196484	0.008299	0.107580	0.125905
12	0.632614	0.026722	0.346372	0.405373
13	66.058685	2.790458	36.168853	42.329833
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.179638	0.007588	0.098356	0.115110
17	0.807959	0.034129	0.442378	0.517733
18	0.171851	0.007259	0.094093	0.110120
19	0.902382	0.038118	0.494078	0.578239
20	0.142074	0.006001	0.077789	0.091040
21	0.071340	0.003013	0.039060	0.045714
22	0.416640	0.017599	0.228121	0.266979
23	0.000000	0.000000	0.000000	0.000000
24	0.060948	0.002574	0.033371	0.039055
25	0.028357	0.001197	0.015526	0.018171
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.166434	0.007030	0.091127	0.106649
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999938	99.999969	4.224208	

CARBON BALANCE 11.644998 LB AT/MOLN2. 101.92 PERCENT
HYDROGEN BALANCE 29.016830 LB AT/MOLN2. 101.58 PERCENT
OXYGEN BALANCE 0.530773 LB AT/MOLN2. 99.83 PERCENT

PERCENT O2 REACT 29.0234 PERCENT C4 REACT 2.3078

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3235	0.1151	0.5312	0.1555	0.7306	0.2402	1.2559	0.5177
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.6089	0.2166	1.0000	0.2926	1.3751	0.4521	2.3640	0.9745
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.3557	1.6420	0.4806	2.2581	0.7424	3.8819	1.6002
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.2701	0.8076	3.7278	1.0911	5.1263	1.6855	8.8126	3.6327

RUN NO = 71 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	2.812016	0.120228	0.825783	0.586532
3	23.388839	1.000000	6.868428	4.878459
4	0.936346	0.040033	0.274970	0.195303
5	0.940811	0.040224	0.276281	0.196235
6	0.857326	0.036655	0.251764	0.178821
7	0.278786	0.011919	0.081869	0.058149
8	0.053351	0.002281	0.015667	0.011128
9	1.321080	0.056483	0.387951	0.275551
10	0.207224	0.008859	0.060854	0.043222
11	0.195730	0.008368	0.057478	0.040825
12	0.981209	0.041952	0.288144	0.204661
13	62.013092	2.651397	18.210929	12.934732
14	0.057907	0.002475	0.017005	0.012078
15	0.035779	0.001529	0.010507	0.007462
16	0.310660	0.013282	0.091229	0.064797
17	2.468503	0.105541	0.724907	0.514882
18	0.253112	0.010821	0.074329	0.052794
19	1.795644	0.076773	0.527313	0.374536
20	0.226163	0.009669	0.066415	0.047173
21	0.089262	0.003816	0.026212	0.018618
22	0.346783	0.014826	0.101837	0.072332
23	0.020699	0.000885	0.006078	0.004317
24	0.075858	0.003243	0.022276	0.015822
25	0.028898	0.001235	0.008486	0.006027
26	0.060266	0.002576	0.017697	0.012570
27	0.044387	0.001897	0.013034	0.009258
28	0.000000	0.000000	0.000000	0.000000
29	0.200421	0.008569	0.058856	0.041804
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999969	99.999984	4.275542	

CARBON BALANCE 11.436744 LB AT/MOLN2. 100.09 PERCENT
HYDROGEN BALANCE 28.598785 LB AT/MOLN2. 100.12 PERCENT
OXYGEN BALANCE 0.546913 LB AT/MOLN2. 102.87 PERCENT

PERCENT O2 REACT 54.7710 PERCENT C4 REACT 7.1763

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1953	0.0647	0.2454	0.2655	0.4475	0.1250	0.6552	0.5148
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.7955	0.2639	1.0000	1.0815	1.8230	0.5093	2.6692	2.0973
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.3317	1.2569	1.3594	2.2914	0.6402	3.3550	2.6363
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.0921	0.3623	1.3728	1.4847	2.5026	0.6992	3.6642	2.8793

DATE	DESCRIPTION	AMOUNT	BALANCE
1	10/1/00	100.00	100.00
2	10/2/00	100.00	200.00
3	10/3/00	100.00	300.00
4	10/4/00	100.00	400.00
5	10/5/00	100.00	500.00
6	10/6/00	100.00	600.00
7	10/7/00	100.00	700.00
8	10/8/00	100.00	800.00
9	10/9/00	100.00	900.00
10	10/10/00	100.00	1000.00
11	10/11/00	100.00	1100.00
12	10/12/00	100.00	1200.00
13	10/13/00	100.00	1300.00
14	10/14/00	100.00	1400.00
15	10/15/00	100.00	1500.00
16	10/16/00	100.00	1600.00
17	10/17/00	100.00	1700.00
18	10/18/00	100.00	1800.00
19	10/19/00	100.00	1900.00
20	10/20/00	100.00	2000.00
21	10/21/00	100.00	2100.00
22	10/22/00	100.00	2200.00
23	10/23/00	100.00	2300.00
24	10/24/00	100.00	2400.00
25	10/25/00	100.00	2500.00
26	10/26/00	100.00	2600.00
27	10/27/00	100.00	2700.00
28	10/28/00	100.00	2800.00
29	10/29/00	100.00	2900.00
30	10/30/00	100.00	3000.00
TOTAL			3000.00

DATE	DESCRIPTION	AMOUNT	BALANCE
10/1/00	100.00	100.00	100.00
10/2/00	100.00	200.00	200.00
10/3/00	100.00	300.00	300.00
10/4/00	100.00	400.00	400.00
10/5/00	100.00	500.00	500.00
10/6/00	100.00	600.00	600.00
10/7/00	100.00	700.00	700.00
10/8/00	100.00	800.00	800.00
10/9/00	100.00	900.00	900.00
10/10/00	100.00	1000.00	1000.00
10/11/00	100.00	1100.00	1100.00
10/12/00	100.00	1200.00	1200.00
10/13/00	100.00	1300.00	1300.00
10/14/00	100.00	1400.00	1400.00
10/15/00	100.00	1500.00	1500.00
10/16/00	100.00	1600.00	1600.00
10/17/00	100.00	1700.00	1700.00
10/18/00	100.00	1800.00	1800.00
10/19/00	100.00	1900.00	1900.00
10/20/00	100.00	2000.00	2000.00
10/21/00	100.00	2100.00	2100.00
10/22/00	100.00	2200.00	2200.00
10/23/00	100.00	2300.00	2300.00
10/24/00	100.00	2400.00	2400.00
10/25/00	100.00	2500.00	2500.00
10/26/00	100.00	2600.00	2600.00
10/27/00	100.00	2700.00	2700.00
10/28/00	100.00	2800.00	2800.00
10/29/00	100.00	2900.00	2900.00
10/30/00	100.00	3000.00	3000.00

RUN NO = 71 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	1.377619	0.057874	0.278309	0.207748
3	23.803764	1.000000	4.808878	3.589667
4	1.368247	0.057480	0.276415	0.206335
5	0.970703	0.040779	0.196103	0.146384
6	0.880527	0.036991	0.177885	0.132785
7	0.327966	0.013777	0.066256	0.049458
8	0.096843	0.004068	0.019564	0.014604
9	0.528137	0.022187	0.106695	0.079644
10	0.166692	0.007002	0.033675	0.025137
11	0.242745	0.010197	0.049039	0.036606
12	1.484827	0.062377	0.299967	0.223915
13	61.361396	2.577802	12.396339	9.253454
14	0.046247	0.001942	0.009343	0.006974
15	0.046247	0.001942	0.009343	0.006974
16	0.239803	0.010074	0.048445	0.036162
17	3.051688	0.128201	0.616507	0.460202
18	0.263576	0.011072	0.053248	0.039748
19	2.269981	0.095362	0.458585	0.342318
20	0.344065	0.014454	0.069508	0.051885
21	0.039928	0.001677	0.008066	0.006021
22	0.448308	0.018833	0.090568	0.067606
23	0.050191	0.002108	0.010139	0.007568
24	0.151750	0.006375	0.030656	0.022884
25	0.051257	0.002153	0.010355	0.007729
26	0.071113	0.002987	0.014366	0.010724
27	0.050699	0.002129	0.010242	0.007645
28	0.044181	0.001856	0.008925	0.006662
29	0.221654	0.009311	0.044779	0.033426
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999969	100.000015	4.201014
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CARBON BALANCE	11.207918 LB AT/MOLN2.	98.09 PERCENT
HYDROGEN BALANCE	28.052299 LB AT/MOLN2.	98.20 PERCENT
OXYGEN BALANCE	0.489900 LB AT/MOLN2.	92.14 PERCENT

PERCENT O2 REACT	78.2283	PERCENT C4 REACT	9.7528
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2063	0.0361	0.2605	0.2104	0.3924	0.1221	0.6042	0.4602
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.7920	0.1388	1.0000	0.8077	1.5065	0.4689	2.3192	1.7664
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1752	1.2626	1.0199	1.9021	0.5920	2.9283	2.2303
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.5538	0.2723	1.9619	1.5848	2.9558	0.9200	4.5503	3.4657

JOYCE HALL	0.68000 LB TAVOLAS	85.14
HAYDGEN HALL	5.8.02300 LB TAVOLAS	91.50
LEAFHOLD	11.50000 LB TAVOLAS	91.50

RUN NO = 71 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	0.558882	0.023423	0.096629	0.079782
3	23.860351	1.000000	4.125419	3.406154
4	1.872119	0.078461	0.323686	0.267252
5	1.078356	0.045194	0.186446	0.153939
6	1.004668	0.042106	0.173705	0.143420
7	0.343382	0.014391	0.059370	0.049019
8	0.119448	0.005006	0.020652	0.017051
9	0.681931	0.028580	0.117904	0.097348
10	0.159912	0.006702	0.027648	0.022828
11	0.169361	0.007098	0.029282	0.024176
12	1.143559	0.047927	0.197719	0.163247
13	61.149147	2.562793	10.572595	8.729269
14	0.022594	0.000946	0.003906	0.003225
15	0.035493	0.001487	0.006136	0.005066
16	0.339682	0.014236	0.058730	0.048490
17	3.467437	0.145322	0.599514	0.494989
18	0.170752	0.007156	0.029522	0.024375
19	2.153286	0.090245	0.372299	0.307389
20	0.321944	0.013492	0.055663	0.045958
21	0.134343	0.005630	0.023227	0.019178
22	0.564551	0.023660	0.097610	0.080591
23	0.080249	0.003363	0.013875	0.011455
24	0.122932	0.005152	0.021254	0.017549
25	0.095973	0.004022	0.016593	0.013700
26	0.058583	0.002455	0.010128	0.008362
27	0.046446	0.001946	0.008030	0.006630
28	0.035374	0.001482	0.006116	0.005049
29	0.209405	0.008776	0.036205	0.029893
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999938	100.000015	4.191052
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CARBON	BALANCE	11.139190	LB AT/MOLN2.	97.49	PERCENT
HYDROGEN	BALANCE	27.872375	LB AT/MOLN2.	97.57	PERCENT
OXYGEN	BALANCE	0.466486	LB AT/MOLN2.	87.74	PERCENT

PERCENT O2 REACT	91.1884	PERCENT C4 REACT	10.2782
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2672	0.0484	0.1874	0.2200	0.3648	0.0945	0.5701	0.4949
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.4259	0.2587	1.0000	1.1738	1.9465	0.5042	3.0419	2.6410
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1814	0.7013	0.8232	1.3650	0.3536	2.1333	1.8521
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.8634	0.3381	1.3068	1.5340	2.5437	0.6589	3.9752	3.4513

[illegible]

RUN NO = 71 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	0.522892	0.021707	0.088924	0.068419
3	24.087715	1.000000	4.096433	3.151830
4	2.345620	0.097378	0.398903	0.306919
5	0.868589	0.036059	0.147715	0.113653
6	0.789432	0.032773	0.134253	0.103295
7	0.282398	0.011723	0.048025	0.036951
8	0.130337	0.005410	0.022165	0.017054
9	0.471886	0.019590	0.080250	0.061745
10	0.196301	0.008149	0.033383	0.025685
11	0.144585	0.006002	0.024588	0.018918
12	1.298556	0.053909	0.220836	0.169913
13	61.161201	2.539103	10.401268	8.002822
14	0.041956	0.001741	0.007135	0.005489
15	0.020904	0.000867	0.003555	0.002735
16	0.092742	0.003850	0.015772	0.012135
17	2.782578	0.115518	0.473214	0.364094
18	0.687848	0.028555	0.116977	0.090003
19	2.455324	0.101932	0.417560	0.321274
20	0.356067	0.014782	0.060554	0.046590
21	0.159586	0.006625	0.027139	0.020881
22	0.524400	0.021770	0.089181	0.068616
23	0.017015	0.000706	0.002893	0.002226
24	0.153072	0.006354	0.026032	0.020029
25	0.048136	0.001998	0.008186	0.006298
26	0.067485	0.002801	0.011476	0.008830
27	0.031138	0.001292	0.005295	0.004074
28	0.038567	0.001601	0.006558	0.005046
29	0.223763	0.009289	0.038053	0.029278
30	0.000000	0.000000	0.000000	0.000000

TOTALS	100.000015	99.999969	4.151491
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CARBON	BALANCE	11.044004	LB	AT/MOLN2.	96.66	PERCENT
HYDROGEN	BALANCE	27.565601	LB	AT/MOLN2.	96.50	PERCENT
OXYGEN	BALANCE	0.461723	LB	AT/MOLN2.	86.84	PERCENT

PERCENT O2 REACT	91.8337	PERCENT C4 REACT	11.1076
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3069	0.0121	0.1888	0.1676	0.3802	0.1606	0.6231	0.3640
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.6253	0.0642	1.0000	0.8878	2.0137	0.8510	3.3000	1.9281
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.0395	0.6152	0.5462	1.2389	0.5235	2.0303	1.1862
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.9712	0.1174	1.8280	1.6230	3.6813	1.5557	6.0326	3.5247

RUN NO = 73

REACTOR ENTRANCE CONDITIONS

AIR = 2.30 LB/HR BUTANE = 9.20 LB/HR

TEMPERATURE = 678.00 DEG F

PRESSURE = 53.72 LB/SQ IN

OXYGEN = 7.0333 NITROGEN = 26.4589 BUTANE = 66.5076 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.5136 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 9.4559

DENSITY OF GAS MIXTURE = 0.2125 LB/CU FT

GAS VELOCITY = 7.05 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.37 SEC

REYNOLDS NUMBER = 6015

Time = 34

Positional coordinates

1.00 1.00 1.00 1.00 1.00 1.00

1.00 1.00 1.00 1.00 1.00 1.00

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1.00 1.00 1.00 1.00 1.00 1.00

RUN NO = 73 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	6.735735	0.255434	24.589363	12.922405
3	26.369693	1.000000	96.264770	50.589859
4	0.044222	0.001677	0.161437	0.084840
5	0.000000	0.000000	0.000000	0.000000
6	0.011817	0.000448	0.043139	0.022671
7	0.000000	0.000000	0.000000	0.000000
8	0.000000	0.000000	0.000000	0.000000
9	0.538579	0.020424	1.966129	1.033256
10	0.105647	0.004006	0.385675	0.202683
11	0.091110	0.003455	0.332607	0.174794
12	0.021585	0.000818	0.078800	0.041412
13	65.761993	2.493847	240.069610	126.163375
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.059945	0.002273	0.218836	0.115004
17	0.000000	0.000000	0.000000	0.000000
18	0.036274	0.001375	0.132421	0.069591
19	0.077554	0.002941	0.283117	0.148786
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.145901	0.005532	0.532626	0.279910
23	0.000000	0.000000	0.000000	0.000000
24	0.000000	0.000000	0.000000	0.000000
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	099.999999	099.999999	3.792232
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CARBON	BALANCE	10.090005	LB AT/MOLN2.	100.35	PERCENT
HYDROGEN	BALANCE	25.173702	LB AT/MOLN2.	100.14	PERCENT
OXYGEN	BALANCE	0.526942	LB AT/MOLN2.	99.11	PERCENT

PERCENT O2 REACT	3.9078	PERCENT C4 REACT	0.7863
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.0848	0.1150	0.2162	0.0000	0.1487	0.0695	0.4982	0.0000
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.3924	0.5319	1.0000	0.0000	0.6881	0.3218	2.3046	0.0000
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	1.3555	2.5483	0.0000	1.7537	0.8202	5.8732	0.0000
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.7421	5.0727	9.5366	0.0000	6.5627	3.0695	21.9789	0.0000

RUN NO = 73 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.556699	0.212644	3.998744	2.470916
3	26.131362	1.000000	18.804809	11.619922
4	0.289617	0.011083	0.208415	0.128785
5	0.032918	0.001259	0.023688	0.014637
6	0.094639	0.003621	0.068105	0.042083
7	0.000000	0.000000	0.000000	0.000000
8	0.000000	0.000000	0.000000	0.000000
9	1.250891	0.047869	0.900174	0.556238
10	0.071657	0.002742	0.051566	0.031864
11	0.382295	0.014629	0.275109	0.169996
12	0.417984	0.015995	0.300792	0.185866
13	63.435317	2.427555	45.649696	28.208000
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.320952	0.012282	0.230965	0.142719
17	0.262814	0.010057	0.189128	0.116866
18	0.032691	0.001251	0.023525	0.014536
19	0.953552	0.036490	0.686201	0.424019
20	0.079003	0.003023	0.056853	0.035130
21	0.080961	0.003098	0.058261	0.036001
22	0.193152	0.007391	0.138997	0.085889
23	0.051673	0.001977	0.037185	0.022978
24	0.095915	0.003670	0.069023	0.042651
25	0.102211	0.003911	0.073553	0.045450
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.163819	0.006269	0.117888	0.072846
30	0.000000	0.000000	0.000000	0.000000
TOTALS	100.000015	100.000015	3.826820	

CARBON BALANCE 10.137680 LB AT/MOLN2. 100.82 PERCENT
HYDROGEN BALANCE 25.203571 LB AT/MOLN2. 100.26 PERCENT
OXYGEN BALANCE 0.538077 LB AT/MOLN2. 101.20 PERCENT

PERCENT O2 REACT 20.0050 PERCENT C4 REACT 3.4237

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1287	0.1427	0.3558	0.0146	0.5328	0.0923	0.7795	0.1168
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.3618	0.4010	1.0000	0.0411	1.4973	0.2594	2.1904	0.3284
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	1.1081	2.7632	0.1136	4.1376	0.7168	6.0527	0.9074
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.0602	3.3913	8.4560	0.3478	12.6620	2.1936	18.5226	2.7769

RUN NO = 73 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	2.392937	0.089924	0.511229	0.372916
3	26.610538	1.000000	5.685104	4.146995
4	1.179711	0.044332	0.252034	0.183846
5	0.310871	0.011682	0.066414	0.048446
6	0.556060	0.020896	0.118797	0.086656
7	0.100980	0.003794	0.021573	0.015736
8	0.015236	0.000572	0.003255	0.002374
9	1.587761	0.059666	0.339210	0.247437
10	0.062563	0.002351	0.013366	0.009749
11	0.593016	0.022285	0.126692	0.092415
12	1.217253	0.045743	0.260055	0.189697
13	60.471794	2.272475	12.919258	9.423944
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.515825	0.019384	0.110201	0.080386
17	1.290696	0.048503	0.275745	0.201142
18	0.102453	0.003850	0.021888	0.015966
19	1.891610	0.071085	0.404125	0.294789
20	0.373188	0.014024	0.079728	0.058157
21	0.107068	0.004023	0.022874	0.016685
22	0.139964	0.005259	0.029902	0.021812
23	0.069096	0.002596	0.014761	0.010768
24	0.100276	0.003768	0.021423	0.015627
25	0.044567	0.001674	0.009521	0.006945
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.032750	0.001230	0.006996	0.005103
29	0.233905	0.008789	0.049971	0.036451
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999908	100.000015	3.757910	

CARBON BALANCE	9.863891 LB AT/MOLN2.	98.10 PERCENT
HYDROGEN BALANCE	24.448135 LB AT/MOLN2.	97.26 PERCENT
OXYGEN BALANCE	0.427755 LB AT/MOLN2.	80.45 PERCENT

PERCENT O2 REACT	66.1712	PERCENT C4 REACT	9.5932
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1838	0.0803	0.2821	0.0665	0.3479	0.0897	0.4823	0.2011
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.6516	0.2849	1.0000	0.2359	1.2332	0.3181	1.7096	0.7129
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.4372	1.5345	0.3620	1.8924	0.4881	2.6234	1.0940
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.1215	0.9276	3.2555	0.7680	4.0150	1.0357	5.5657	2.3211

DATE: 01/01/2010

DATE	DESCRIPTION	AMOUNT	CHECK NO.	BANK
01/01/2010	OPENING BALANCE	100.00		CHASE
01/02/2010	PAYROLL	50.00	101	CHASE
01/03/2010	RENT	25.00	102	CHASE
01/04/2010	UTILITIES	15.00	103	CHASE
01/05/2010	FOOD	10.00	104	CHASE
01/06/2010	TRANSPORT	20.00	105	CHASE
01/07/2010	INSURANCE	30.00	106	CHASE
01/08/2010	MAINTENANCE	12.00	107	CHASE
01/09/2010	ADVERTISING	18.00	108	CHASE
01/10/2010	TRAVEL	22.00	109	CHASE
01/11/2010	TELEPHONE	8.00	110	CHASE
01/12/2010	POSTAGE	5.00	111	CHASE
01/13/2010	COMPUTER	14.00	112	CHASE
01/14/2010	OFFICE SUPPLIES	9.00	113	CHASE
01/15/2010	SALES TAX	11.00	114	CHASE
01/16/2010	PROPERTY TAX	28.00	115	CHASE
01/17/2010	INCOME TAX	35.00	116	CHASE
01/18/2010	INTEREST	4.00	117	CHASE
01/19/2010	DEPOSITS	10.00	118	CHASE
01/20/2010	SALES	15.00	119	CHASE
01/21/2010	REVENUE	20.00	120	CHASE
01/22/2010	EXPENSES	12.00	121	CHASE
01/23/2010	INVENTORY	18.00	122	CHASE
01/24/2010	ASSETS	22.00	123	CHASE
01/25/2010	LIABILITIES	28.00	124	CHASE
01/26/2010	EQUITY	35.00	125	CHASE
01/27/2010	DEPRECIATION	4.00	126	CHASE
01/28/2010	AMORTIZATION	10.00	127	CHASE
01/29/2010	GOODWILL	15.00	128	CHASE
01/30/2010	INTANGIBLES	20.00	129	CHASE
01/31/2010	CLOSING BALANCE	100.00		CHASE

DATE	DESCRIPTION	AMOUNT	CHECK NO.	BANK
01/01/2010	OPENING BALANCE	100.00		CHASE
01/02/2010	PAYROLL	50.00	101	CHASE
01/03/2010	RENT	25.00	102	CHASE
01/04/2010	UTILITIES	15.00	103	CHASE
01/05/2010	FOOD	10.00	104	CHASE
01/06/2010	TRANSPORT	20.00	105	CHASE
01/07/2010	INSURANCE	30.00	106	CHASE
01/08/2010	MAINTENANCE	12.00	107	CHASE
01/09/2010	ADVERTISING	18.00	108	CHASE
01/10/2010	TRAVEL	22.00	109	CHASE
01/11/2010	TELEPHONE	8.00	110	CHASE
01/12/2010	POSTAGE	5.00	111	CHASE
01/13/2010	COMPUTER	14.00	112	CHASE
01/14/2010	OFFICE SUPPLIES	9.00	113	CHASE
01/15/2010	SALES TAX	11.00	114	CHASE
01/16/2010	PROPERTY TAX	28.00	115	CHASE
01/17/2010	INCOME TAX	35.00	116	CHASE
01/18/2010	INTEREST	4.00	117	CHASE
01/19/2010	DEPOSITS	10.00	118	CHASE
01/20/2010	SALES	15.00	119	CHASE
01/21/2010	REVENUE	20.00	120	CHASE
01/22/2010	EXPENSES	12.00	121	CHASE
01/23/2010	INVENTORY	18.00	122	CHASE
01/24/2010	ASSETS	22.00	123	CHASE
01/25/2010	LIABILITIES	28.00	124	CHASE
01/26/2010	EQUITY	35.00	125	CHASE
01/27/2010	DEPRECIATION	4.00	126	CHASE
01/28/2010	AMORTIZATION	10.00	127	CHASE
01/29/2010	GOODWILL	15.00	128	CHASE
01/30/2010	INTANGIBLES	20.00	129	CHASE
01/31/2010	CLOSING BALANCE	100.00		CHASE

DATE	DESCRIPTION	AMOUNT	CHECK NO.	BANK
01/01/2010	OPENING BALANCE	100.00		CHASE
01/02/2010	PAYROLL	50.00	101	CHASE
01/03/2010	RENT	25.00	102	CHASE
01/04/2010	UTILITIES	15.00	103	CHASE
01/05/2010	FOOD	10.00	104	CHASE
01/06/2010	TRANSPORT	20.00	105	CHASE
01/07/2010	INSURANCE	30.00	106	CHASE
01/08/2010	MAINTENANCE	12.00	107	CHASE
01/09/2010	ADVERTISING	18.00	108	CHASE
01/10/2010	TRAVEL	22.00	109	CHASE
01/11/2010	TELEPHONE	8.00	110	CHASE
01/12/2010	POSTAGE	5.00	111	CHASE
01/13/2010	COMPUTER	14.00	112	CHASE
01/14/2010	OFFICE SUPPLIES	9.00	113	CHASE
01/15/2010	SALES TAX	11.00	114	CHASE
01/16/2010	PROPERTY TAX	28.00	115	CHASE
01/17/2010	INCOME TAX	35.00	116	CHASE
01/18/2010	INTEREST	4.00	117	CHASE
01/19/2010	DEPOSITS	10.00	118	CHASE
01/20/2010	SALES	15.00	119	CHASE
01/21/2010	REVENUE	20.00	120	CHASE
01/22/2010	EXPENSES	12.00	121	CHASE
01/23/2010	INVENTORY	18.00	122	CHASE
01/24/2010	ASSETS	22.00	123	CHASE
01/25/2010	LIABILITIES	28.00	124	CHASE
01/26/2010	EQUITY	35.00	125	CHASE
01/27/2010	DEPRECIATION	4.00	126	CHASE
01/28/2010	AMORTIZATION	10.00	127	CHASE
01/29/2010	GOODWILL	15.00	128	CHASE
01/30/2010	INTANGIBLES	20.00	129	CHASE
01/31/2010	CLOSING BALANCE	100.00		CHASE

RUN NO = 73 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	0.298470	0.011151	0.043787	0.031957
3	26.765254	1.000000	3.926630	2.865784
4	1.899742	0.070977	0.278704	0.203407
5	0.640388	0.023926	0.093948	0.068567
6	0.776641	0.029016	0.113938	0.083155
7	0.147730	0.005519	0.021672	0.015817
8	0.045277	0.001691	0.006642	0.004847
9	0.910947	0.034034	0.133641	0.097536
10	0.061014	0.002279	0.008951	0.006532
11	0.320185	0.011962	0.046973	0.034282
12	1.585602	0.059241	0.232617	0.169772
13	57.937927	2.164669	8.499856	6.203474
14	0.040361	0.001507	0.005921	0.004321
15	0.025413	0.000949	0.003728	0.002721
16	0.480291	0.017944	0.070461	0.051425
17	2.664578	0.099553	0.390910	0.285299
18	0.179289	0.006698	0.026302	0.019196
19	3.082465	0.115166	0.452217	0.330042
20	0.732210	0.027356	0.107419	0.078398
21	0.119944	0.004481	0.017596	0.012842
22	0.377981	0.014122	0.055452	0.040470
23	0.179093	0.006691	0.026274	0.019175
24	0.203561	0.007605	0.029863	0.021795
25	0.080566	0.003010	0.011819	0.008626
26	0.045129	0.001686	0.006620	0.004832
27	0.033384	0.001247	0.004897	0.003574
28	0.103811	0.003878	0.015229	0.011115
29	0.262953	0.009824	0.038576	0.028154
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999969	100.000061	3.736191	

CARBON BALANCE	9.586923 LB AT/MOLN2.	95.34 PERCENT
HYDROGEN BALANCE	23.862388 LB AT/MOLN2.	94.93 PERCENT
OXYGEN BALANCE	0.430492 LB AT/MOLN2.	80.97 PERCENT

PERCENT O2 REACT	95.8049	PERCENT C4 REACT	13.8821
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2034	0.0514	0.2040	0.0892	0.3758	0.1229	0.5782	0.2852
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.9968	0.2520	1.0000	0.4372	1.8420	0.6026	2.8336	1.3981
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2528	1.0031	0.4386	1.8478	0.6045	2.8426	1.4026
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.4461	0.6184	2.4538	1.0730	4.5200	1.4787	6.9535	3.4308

RUN NO = 73 SAMPLE NO = 5

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	0.426611	0.016119	0.064556	0.055832
3	26.464939	1.000000	4.004760	3.463556
4	3.130710	0.118296	0.473749	0.409726
5	0.608912	0.023008	0.092142	0.079690
6	0.747669	0.028251	0.113139	0.097850
7	0.178775	0.006755	0.027052	0.023396
8	0.081326	0.003072	0.012306	0.010643
9	0.809831	0.030600	0.122546	0.105985
10	0.085166	0.003218	0.012887	0.011146
11	0.202320	0.007644	0.030615	0.026478
12	1.316199	0.049733	0.199171	0.172255
13	58.881668	2.224893	8.910165	7.706042
14	0.036950	0.001396	0.005591	0.004835
15	0.018475	0.000698	0.002795	0.002417
16	0.472850	0.017867	0.071553	0.061883
17	2.531255	0.095645	0.383037	0.331273
18	0.127096	0.004802	0.019232	0.016633
19	2.191590	0.082811	0.331638	0.286820
20	0.556666	0.021034	0.084236	0.072852
21	0.089005	0.003363	0.013468	0.011648
22	0.316660	0.011965	0.047918	0.041442
23	0.124063	0.004687	0.018773	0.016236
24	0.153979	0.005818	0.023300	0.020151
25	0.053347	0.002015	0.008072	0.006981
26	0.075747	0.002862	0.011462	0.009913
27	0.019706	0.000744	0.002982	0.002579
28	0.064150	0.002423	0.009707	0.008395
29	0.234533	0.008862	0.035490	0.030694
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999908	100.000076	3.778587
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CARBON BALANCE	9.738262 LB AT/MOLN2.	96.85 PERCENT
HYDROGEN BALANCE	24.119789 LB AT/MOLN2.	95.95 PERCENT
OXYGEN BALANCE	0.433306 LB AT/MOLN2.	81.50 PERCENT

PERCENT O2 REACT	93.9358	PERCENT C4 REACT	11.4862
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.4097	0.0618	0.1987	0.1137	0.3390	0.1122	0.5243	0.3312
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
2.0616	0.3113	1.0000	0.5722	1.7061	0.5646	2.6384	1.6669
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1510	0.4850	0.2775	0.8275	0.2738	1.2797	0.8085
	MOLE	PRODUCT	PER MOLE	ETHENE			
4.1872	0.6324	2.0310	1.1622	3.4652	1.1468	5.3587	3.3855

RUN NO = 75

REACTOR ENTRANCE CONDITIONS

AIR = 2.30 LB/HR BUTANE = 8.20 LB/HR

TEMPERATURE = 655.00 DEG F

PRESSURE = 51.35 LB/SQ IN

OXYGEN = 7.5814 NITROGEN = 28.5207 BUTANE = 63.8977 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 2.2403 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 8.4281

DENSITY OF GAS MIXTURE = 0.2041 LB/CU FT

GAS VELOCITY = 6.70 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.44 SEC

REYNOLDS NUMBER = 5492

THE END

RECEIVED

DATE = 10/10/10

TEMPERATURE = 22.00 C

RESISTANCE = 10.00 K

WATER = 1.000 W/100 G

WATER = 1.000 W/100 G

WATER TO WATER RATIO = 1.000

WATER TO WATER RATIO = 1.000

WATER TO WATER RATIO = 1.000

WATER TO WATER RATIO = 1.000

WATER TO WATER RATIO = 1.000

RUN NO = 75 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	7.120763	0.251145	17.110580	49.842842
3	28.353195	1.000000	68.130279	198.462402
4	0.056273	0.001984	0.135220	0.393894
5	0.000000	0.000000	0.000000	0.000000
6	0.001870	0.000065	0.004494	0.013093
7	0.000000	0.000000	0.000000	0.000000
8	0.000000	0.000000	0.000000	0.000000
9	0.557253	0.019653	1.339030	3.900575
10	0.070625	0.002490	0.169707	0.494354
11	0.077118	0.002719	0.185308	0.539800
12	0.006577	0.000231	0.015805	0.046039
13	63.379486	2.235356	152.295410	443.634094
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.323609	0.011413	0.777605	2.265152
17	0.000000	0.000000	0.000000	0.000000
18	0.000000	0.000000	0.000000	0.000000
19	0.053254	0.001878	0.127965	0.372762
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.000000	0.000000	0.000000	0.000000
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999984	100.000015	3.526938	

CARBON BALANCE 9.037563 LB AT/MOLN2. 100.84 PERCENT
HYDROGEN BALANCE 22.527782 LB AT/MOLN2. 100.55 PERCENT
OXYGEN BALANCE 0.528979 LB AT/MOLN2. 99.49 PERCENT

PERCENT O2 REACT 5.5216 PERCENT C4 REACT 0.2249

CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3938	2.2651	0.5858	0.0000	0.3727	0.0000	0.3727	0.0000
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.6723	3.8665	1.0000	0.0000	0.6362	0.0000	0.6362	0.0000
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	5.7506	1.4873	0.0000	0.9463	0.0000	0.9463	0.0000
	MOLE	PRODUCT	PER MOLE	ETHENE			
30.0835173	0.0000	44.7432	0.0000	28.4695	0.0000	28.4695	0.0000

RUN NO = 75 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	6.801396	0.238518	8.735589	5.877558
3	28.515167	1.000000	36.624359	24.641937
4	0.084489	0.002962	0.108516	0.073013
5	0.000000	0.000000	0.000000	0.000000
6	0.015748	0.000552	0.020227	0.013609
7	0.000000	0.000000	0.000000	0.000000
8	0.000000	0.000000	0.000000	0.000000
9	0.798050	0.027986	1.025001	0.689650
10	0.066332	0.002326	0.085195	0.057322
11	0.289788	0.010162	0.372198	0.250426
12	0.045770	0.001605	0.058787	0.039553
13	62.728050	2.199813	80.566757	54.207664
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.128227	0.004496	0.164693	0.110810
17	0.032321	0.001133	0.041513	0.027931
18	0.000000	0.000000	0.000000	0.000000
19	0.252670	0.008860	0.324525	0.218350
20	0.000000	0.000000	0.000000	0.000000
21	0.000000	0.000000	0.000000	0.000000
22	0.089461	0.003137	0.114902	0.077309
23	0.072817	0.002553	0.093525	0.062926
24	0.046967	0.001647	0.060323	0.040587
25	0.000000	0.000000	0.000000	0.000000
26	0.032825	0.001151	0.042160	0.028366
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999969	100.000045	3.506906	

CARBON	BALANCE	8.979339 LB AT/MOLN2.	100.19 PERCENT
HYDROGEN	BALANCE	22.370330 LB AT/MOLN2.	99.84 PERCENT
OXYGEN	BALANCE	0.507477 LB AT/MOLN2.	95.45 PERCENT

PERCENT O2 REACT	10.2715	PERCENT C4 REACT	1.8113
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.0730	0.1108	0.2899	0.0000	0.2467	0.0405	0.4275	0.0279
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.2517	0.3821	1.0000	0.0000	0.8508	0.1399	1.4743	0.0963
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	1.5176	3.9716	0.0000	3.3790	0.5558	5.8556	0.3825
	MOLE	PRODUCT	PER MOLE	ETHENE			
5.3647	8.1420	21.3068	0.0000	18.1280	2.9822	31.4143	2.0523

RUN NO = 75 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.997882	0.210000	3.761904	4.633078
3	28.561347	1.000000	17.913833	22.062282
4	0.301833	0.010567	0.189311	0.233151
5	0.038826	0.001359	0.024352	0.029991
6	0.069160	0.002421	0.043377	0.053423
7	0.008222	0.000287	0.005156	0.006351
8	0.000000	0.000000	0.000000	0.000000
9	0.525550	0.018400	0.329628	0.405962
10	0.061365	0.002148	0.038488	0.047401
11	0.188870	0.006612	0.118460	0.145893
12	0.178784	0.006259	0.112134	0.138102
13	62.694122	2.195068	39.322090	48.428215
14	0.039936	0.001398	0.025048	0.030848
15	0.037440	0.001310	0.023482	0.028920
16	0.212941	0.007455	0.133558	0.164487
17	0.025362	0.000888	0.015907	0.019591
18	0.030726	0.001075	0.019272	0.023735
19	0.660023	0.023108	0.413970	0.509837
20	0.061279	0.002145	0.038434	0.047335
21	0.040925	0.001432	0.025668	0.031613
22	0.059096	0.002069	0.037065	0.045649
23	0.040023	0.001401	0.025102	0.030916
24	0.047502	0.001663	0.029793	0.036693
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.118918	0.004163	0.074586	0.091858
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999969	100.000015	3.501236	

CARBON	BALANCE	8.993825 LB AT/MOLN2.	100.35 PERCENT
HYDROGEN	BALANCE	22.405612 LB AT/MOLN2.	100.00 PERCENT
OXYGEN	BALANCE	0.483427 LB AT/MOLN2.	90.93 PERCENT

PERCENT O2 REACT	21.0000	PERCENT C4 REACT	2.0231
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.2331	0.1644	0.2839	0.0363	0.5414	0.1996	0.8176	0.0195
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.8209	0.5791	1.0000	0.1279	1.9065	0.7029	2.8790	0.0689
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.7054	1.2180	0.1558	2.3223	0.8561	3.5068	0.0840
	MOLE	PRODUCT	PER MOLE	ETHENE			
4.3642	3.0789	5.3159	0.6802	10.1351	3.7366	15.3049	0.3667

TABLE 1. - SUMMARY OF DATA

DATE	TIME	WIND	WAVE	WAVE
1	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000	0.0000
19	0.0000	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000
23	0.0000	0.0000	0.0000	0.0000
24	0.0000	0.0000	0.0000	0.0000
25	0.0000	0.0000	0.0000	0.0000
26	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0000
30	0.0000	0.0000	0.0000	0.0000
TOTAL	99.9999	100.0000	99.9999	99.9999

DATE	TIME	WIND	WAVE	WAVE
1	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000	0.0000
19	0.0000	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000
23	0.0000	0.0000	0.0000	0.0000
24	0.0000	0.0000	0.0000	0.0000
25	0.0000	0.0000	0.0000	0.0000
26	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0000
30	0.0000	0.0000	0.0000	0.0000
TOTAL	99.9999	100.0000	99.9999	99.9999

RUN NO = 75 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	3.221381	0.110198	0.708100	0.526986
3	29.232658	1.000000	6.425713	4.782177
4	0.904475	0.030940	0.198815	0.147963
5	0.207886	0.007111	0.045696	0.034008
6	0.228070	0.007801	0.050132	0.037310
7	0.066546	0.002276	0.014627	0.010886
8	0.000000	0.000000	0.000000	0.000000
9	0.766624	0.026224	0.168513	0.125412
10	0.050939	0.001742	0.011197	0.008333
11	0.277616	0.009496	0.061023	0.045415
12	0.724510	0.024784	0.159256	0.118522
13	59.379867	2.031285	13.052453	9.713964
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.287354	0.009829	0.063164	0.047008
17	1.341826	0.045901	0.294950	0.219509
18	0.066016	0.002258	0.014511	0.010799
19	2.322640	0.079453	0.510546	0.379961
20	0.194223	0.006644	0.042692	0.031773
21	0.078958	0.002701	0.017356	0.012916
22	0.070001	0.002394	0.015387	0.011451
23	0.046546	0.001592	0.010231	0.007614
24	0.091373	0.003125	0.020085	0.014947
25	0.058413	0.001998	0.012840	0.009555
26	0.000000	0.000000	0.000000	0.000000
27	0.099009	0.003386	0.021763	0.016196
28	0.000000	0.000000	0.000000	0.000000
29	0.283168	0.009686	0.062244	0.046323
30	0.000000	0.000000	0.000000	0.000000

TOTALS	099.999999	99.999984	3.420831
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CARBON BALANCE	8.593570 LB AT/MOLN2.	95.89 PERCENT
HYDROGEN BALANCE	21.465919 LB AT/MOLN2.	95.81 PERCENT
OXYGEN BALANCE	0.430139 LB AT/MOLN2.	80.90 PERCENT

PERCENT O2 REACT	58.5445	PERCENT C4 REACT	9.3336
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1479	0.0470	0.1639	0.0448	0.4392	0.0737	0.5415	0.2195
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.9025	0.2867	1.0000	0.2738	2.6790	0.4496	3.3033	1.3389
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.3177	1.1079	0.3034	2.9683	0.4982	3.6599	1.4835
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.9657	1.2599	4.3939	1.2032	11.7716	1.9758	14.5145	5.8833

DATE: 11/11/2011 TIME: 11:11

ITEM NO.	ITEM DESCRIPTION	QUANTITY	UNIT	PRICE	TOTAL
1
2
3
4
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29
30
TOTAL					...

ITEM NO.	ITEM DESCRIPTION	QUANTITY	UNIT	PRICE	TOTAL
31
32
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45
46
47
48
49
50

RUN NO = 77

REACTOR ENTRANCE CONDITIONS

AIR = 2.95 LB/HR

BUTANE = 9.20 LB/HR

TEMPERATURE = 650.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 8.2410 NITROGEN = 31.0020 BUTANE = 60.7568 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 1.9597 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 7.3724

DENSITY OF GAS MIXTURE = 0.2094 LB/CU FT

GAS VELOCITY = 7.56 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.27 SEC

REYNOLDS NUMBER = 6245

Run No. 11

Reaction Environmental Conditions

Air = 2.25 L/min Water = 2.00 L/min

Temperature = 60.00 °C

Pressure = 33.00 L/min

Oxygen = 0.250 L/min Nitrogen = 0.250 L/min

Flow = 0.500 L/min Total Flow = 1.000 L/min

Substrate to Water Ratio = 1.00

Density of Gas Mixture = 0.500 g/L

Gas Velocity = 1.00 ft/sec

Residence Time based on Ethanol Conversion = 1.0 sec

Reynolds Number = 2500

RUN NO = 77 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	7.112522	0.229974	6.415313	26.060001
3	30.927375	1.000000	27.895706	113.316696
4	0.119993	0.003879	0.108231	0.439651
5	0.020677	0.000668	0.018650	0.075759
6	0.029383	0.000950	0.026502	0.107658
7	0.003771	0.000121	0.003401	0.013817
8	0.000000	0.000000	0.000000	0.000000
9	0.689704	0.022300	0.622096	2.527051
10	0.057332	0.001853	0.051712	0.210065
11	0.034086	0.001102	0.030745	0.124891
12	0.089453	0.002892	0.080685	0.327755
13	60.337524	1.950942	54.422904	221.074310
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	0.100540	0.003250	0.090685	0.368377
17	0.068359	0.002210	0.061658	0.250466
18	0.020264	0.000655	0.018277	0.074247
19	0.310263	0.010032	0.279850	1.136794
20	0.023227	0.000751	0.020950	0.085105
21	0.028877	0.000933	0.026047	0.105806
22	0.000000	0.000000	0.000000	0.000000
23	0.000000	0.000000	0.000000	0.000000
24	0.026711	0.000863	0.024093	0.097871
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	099.999999	099.999999	3.233381
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CARBON BALANCE	7.920653 LB AT/MOLN2.	101.04 PERCENT
HYDROGEN BALANCE	19.760559 LB AT/MOLN2.	100.83 PERCENT
OXYGEN BALANCE	0.485777 LB AT/MOLN2.	91.37 PERCENT

PERCENT O2 REACT	13.4856	PERCENT C4 REACT	0.4502
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.4396	0.3683	0.4526	0.0895	1.2426	0.2572	1.4998	0.2504
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.9712	0.8138	1.0000	0.1978	2.7451	0.5682	3.3134	0.5533
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.8378	1.0295	0.2037	2.8263	0.5850	3.4113	0.5696
	MOLE	PRODUCT	PER MOLE	ETHENE			
4.0837	3.4217	4.2044	0.8320	11.5420	2.3892	13.9313	2.3264

RUN NO = 77 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.410458	0.177373	2.005373	1.800372
3	30.503177	1.000000	11.305929	10.150171
4	0.363894	0.011929	0.134876	0.121088
5	0.407239	0.013350	0.150942	0.135512
6	0.413784	0.013565	0.153368	0.137689
7	0.113274	0.003713	0.041984	0.037692
8	0.008592	0.000281	0.003184	0.002859
9	1.157999	0.037963	0.429209	0.385333
10	0.037460	0.001228	0.013884	0.012465
11	0.201299	0.006599	0.074611	0.066984
12	0.677830	0.022221	0.251236	0.225553
13	56.773933	1.861246	21.043117	18.891967
14	0.013297	0.000435	0.004928	0.004424
15	0.012466	0.000408	0.004620	0.004148
16	0.354879	0.011634	0.131535	0.118089
17	1.196382	0.039221	0.443436	0.398105
18	0.040924	0.001341	0.015168	0.013617
19	1.571241	0.051510	0.582376	0.522842
20	0.344003	0.011277	0.127503	0.114469
21	0.022462	0.000736	0.008325	0.007474
22	0.022997	0.000753	0.008523	0.007652
23	0.034500	0.001131	0.012787	0.011480
24	0.077884	0.002553	0.028867	0.025916
25	0.059340	0.001945	0.021994	0.019746
26	0.005352	0.000175	0.001983	0.001781
27	0.003368	0.000110	0.001248	0.001120
28	0.005276	0.000172	0.001955	0.001755
29	0.166843	0.005469	0.061840	0.055518
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999954	100.000030	3.278346
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CARBON	BALANCE	7.874156	LB AT/MOLN2.	100.44	PERCENT
HYDROGEN	BALANCE	19.656898	LB AT/MOLN2.	100.30	PERCENT
OXYGEN	BALANCE	0.506345	LB AT/MOLN2.	95.24	PERCENT

PERCENT O2 REACT	33.2737	PERCENT C4 REACT	5.0271
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1210	0.1180	0.2925	0.1760	0.5876	0.1551	0.7833	0.3981
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.4139	0.4036	1.0000	0.6018	2.0086	0.5302	2.6778	1.3608
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.9752	2.4158	1.4540	4.8527	1.2810	6.4694	3.2877
	MOLE	PRODUCT	PER MOLE	ETHENE			
0.8794	0.8576	2.1246	1.2786	4.2676	1.1266	5.6894	2.8913

DATE: 11/15/1977

DATE	DESCRIPTION	AMOUNT	BALANCE
11/15/77	100.00	100.00	100.00
11/16/77	10.00	90.00	90.00
11/17/77	20.00	70.00	70.00
11/18/77	15.00	55.00	55.00
11/19/77	10.00	45.00	45.00
11/20/77	5.00	40.00	40.00
11/21/77	10.00	30.00	30.00
11/22/77	15.00	15.00	15.00
11/23/77	10.00	5.00	5.00
11/24/77	5.00	0.00	0.00
11/25/77	10.00	10.00	10.00
11/26/77	15.00	25.00	25.00
11/27/77	10.00	15.00	15.00
11/28/77	5.00	10.00	10.00
11/29/77	10.00	20.00	20.00
11/30/77	15.00	35.00	35.00
12/01/77	10.00	25.00	25.00
12/02/77	5.00	20.00	20.00
12/03/77	10.00	10.00	10.00
12/04/77	15.00	25.00	25.00
12/05/77	10.00	15.00	15.00
12/06/77	5.00	10.00	10.00
12/07/77	10.00	20.00	20.00
12/08/77	15.00	35.00	35.00
12/09/77	10.00	25.00	25.00
12/10/77	5.00	20.00	20.00
12/11/77	10.00	10.00	10.00
12/12/77	15.00	25.00	25.00
12/13/77	10.00	15.00	15.00
12/14/77	5.00	10.00	10.00
12/15/77	10.00	20.00	20.00
12/16/77	15.00	35.00	35.00
12/17/77	10.00	25.00	25.00
12/18/77	5.00	20.00	20.00
12/19/77	10.00	10.00	10.00
12/20/77	15.00	25.00	25.00
12/21/77	10.00	15.00	15.00
12/22/77	5.00	10.00	10.00
12/23/77	10.00	20.00	20.00
12/24/77	15.00	35.00	35.00
12/25/77	10.00	25.00	25.00
12/26/77	5.00	20.00	20.00
12/27/77	10.00	10.00	10.00
12/28/77	15.00	25.00	25.00
12/29/77	10.00	15.00	15.00
12/30/77	5.00	10.00	10.00
12/31/77	10.00	20.00	20.00
12/32/77	15.00	35.00	35.00
12/33/77	10.00	25.00	25.00
12/34/77	5.00	20.00	20.00
12/35/77	10.00	10.00	10.00
12/36/77	15.00	25.00	25.00
12/37/77	10.00	15.00	15.00
12/38/77	5.00	10.00	10.00
12/39/77	10.00	20.00	20.00
12/40/77	15.00	35.00	35.00
12/41/77	10.00	25.00	25.00
12/42/77	5.00	20.00	20.00
12/43/77	10.00	10.00	10.00
12/44/77	15.00	25.00	25.00
12/45/77	10.00	15.00	15.00
12/46/77	5.00	10.00	10.00
12/47/77	10.00	20.00	20.00
12/48/77	15.00	35.00	35.00
12/49/77	10.00	25.00	25.00
12/50/77	5.00	20.00	20.00
12/51/77	10.00	10.00	10.00
12/52/77	15.00	25.00	25.00
12/53/77	10.00	15.00	15.00
12/54/77	5.00	10.00	10.00
12/55/77	10.00	20.00	20.00
12/56/77	15.00	35.00	35.00
12/57/77	10.00	25.00	25.00
12/58/77	5.00	20.00	20.00
12/59/77	10.00	10.00	10.00
12/60/77	15.00	25.00	25.00
12/61/77	10.00	15.00	15.00
12/62/77	5.00	10.00	10.00
12/63/77	10.00	20.00	20.00
12/64/77	15.00	35.00	35.00
12/65/77	10.00	25.00	25.00
12/66/77	5.00	20.00	20.00
12/67/77	10.00	10.00	10.00
12/68/77	15.00	25.00	25.00
12/69/77	10.00	15.00	15.00
12/70/77	5.00	10.00	10.00
12/71/77	10.00	20.00	20.00
12/72/77	15.00	35.00	35.00
12/73/77	10.00	25.00	25.00
12/74/77	5.00	20.00	20.00
12/75/77	10.00	10.00	10.00
12/76/77	15.00	25.00	25.00
12/77/77	10.00	15.00	15.00
12/78/77	5.00	10.00	10.00
12/79/77	10.00	20.00	20.00
12/80/77	15.00	35.00	35.00
12/81/77	10.00	25.00	25.00
12/82/77	5.00	20.00	20.00
12/83/77	10.00	10.00	10.00
12/84/77	15.00	25.00	25.00
12/85/77	10.00	15.00	15.00
12/86/77	5.00	10.00	10.00
12/87/77	10.00	20.00	20.00
12/88/77	15.00	35.00	35.00
12/89/77	10.00	25.00	25.00
12/90/77	5.00	20.00	20.00
12/91/77	10.00	10.00	10.00
12/92/77	15.00	25.00	25.00
12/93/77	10.00	15.00	15.00
12/94/77	5.00	10.00	10.00
12/95/77	10.00	20.00	20.00
12/96/77	15.00	35.00	35.00
12/97/77	10.00	25.00	25.00
12/98/77	5.00	20.00	20.00
12/99/77	10.00	10.00	10.00
12/100/77	15.00	25.00	25.00
12/101/77	10.00	15.00	15.00
12/102/77	5.00	10.00	10.00
12/103/77	10.00	20.00	20.00
12/104/77	15.00	35.00	35.00
12/105/77	10.00	25.00	25.00
12/106/77	5.00	20.00	20.00
12/107/77	10.00	10.00	10.00
12/108/77	15.00	25.00	25.00
12/109/77	10.00	15.00	15.00
12/110/77	5.00	10.00	10.00
12/111/77	10.00	20.00	20.00
12/112/77	15.00	35.00	35.00
12/113/77	10.00	25.00	25.00
12/114/77	5.00	20.00	20.00
12/115/77	10.00	10.00	10.00
12/116/77	15.00	25.00	25.00
12/117/77	10.00	15.00	15.00
12/118/77	5.00	10.00	10.00
12/119/77	10.00	20.00	20.00
12/120/77	15.00	35.00	35.00
12/121/77	10.00	25.00	25.00
12/122/77	5.00	20.00	20.00
12/123/77	10.00	10.00	10.00
12/124/77	15.00	25.00	25.00
12/125/77	10.00	15.00	15.00
12/126/77	5.00	10.00	10.00
12/127/77	10.00	20.00	20.00
12/128/77	15.00	35.00	35.00
12/129/77	10.00	25.00	25.00
12/130/77	5.00	20.00	20.00
12/131/77	10.00	10.00	10.00
12/132/77	15.00	25.00	25.00
12/133/77	10.00	15.00	15.00
12/134/77	5.00	10.00	10.00
12/135/77	10.00	20.00	20.00
12/136/77	15.00	35.00	35.00
12/137/77	10.00	25.00	25.00
12/138/77	5.00	20.00	20.00
12/139/77	10.00	10.00	10.00
12/140/77	15.00	25.00	25.00
12/141/77	10.00	15.00	15.00
12/142/77	5.00	10.00	10.00
12/143/77	10.00	20.00	20.00
12/144/77	15.00	35.00	35.00
12/145/77	10.00	25.00	25.00
12/146/77	5.00	20.00	20.00
12/147/77	10.00	10.00	10.00
12/148/77	15.00	25.00	25.00
12/149/77	10.00	15.00	15.00
12/150/77	5.00	10.00	10.00
12/151/77	10.00	20.00	20.00
12/152/77	15.00	35.00	35.00
12/153/77	10.00	25.00	25.00
12/154/77	5.00	20.00	20.00
12/155/77	10.00	10.00	10.00
12/156/77	15.00	25.00	25.00
12/157/77	10.00	15.00	15.00
12/158/77	5.00	10.00	10.00
12/159/77	10.00	20.00	20.00
12/160/77	15.00	35.00	35.00
12/161/77	10.00	25.00	25.00
12/162/77	5.00	20.00	20.00
12/163/77	10.00	10.00	10.00
12/164/77	15.00	25.00	25.00
12/165/77	10.00	15.00	15.00
12/166/77	5.00	10.00	10.00
12/167/77	10.00	20.00	20.00
12/168/77	15.00	35.00	35.00
12/169/77	10.00	25.00	25.00
12/170/77	5.00	20.00	20.00
12/171/77	10.00	10.00	10.00
12/172/77	15.00	25.00	25.00
12/173/77	10.00	15.00	15.00
12/174/77	5.00	10.00	10.00
12/175/77	10.00	20.00	20.00
12/176/77	15.00	35.00	35.00
12/177/77	10.00	25.00	25.00
12/178/77	5.00	20.00	20.00
12/179/77	10.00	10.00	10.00
12/180/77	15.00	25.00	25.00
12/181/77	10.00	15.00	15.00
12/182/77	5.00	10.00	10.00
12/183/77	10.00	20.00	20.00
12/184/77	15.00	35.00	35.00
12/185/77	10.00	25.00	25.00
12/186/77	5.00	20.00	20.00
12/187/77	10.00	10.00	10.00
12/188/77	15.00	25.00	25.00
12/189/77	10.00	15.00	15.00
12/190/77	5.00	10.00	10.00
12/191/77	10.00	20.00	20.00
12/192/77	15.00	35.00	35.00
12/193/77	10.00	25.00	25.00
12/194/77	5.00	20.00	20.00
12/195/77	10.00	10.00	10.00
12/196/77	15.00	25.00	25.00
12/197/77	10.00	15.00	15.00
12/198/77	5.00	10.00	10.00
12/199/77	10.00	20.00	20.00
12/200/77	15.00	35.00	35.00

TOTAL 100.00000 100.00000 100.00000

HYDROGEN BALANCE 100.00000
OXYGEN BALANCE 100.00000
CARBON BALANCE 100.00000

PERCENT OF REACT 100.00000 100.00000 100.00000

CO	CO2	CH4	ETHANE	ETHYLENE	ACETYLENE	PROPANE	PROPYLENE	BUTANE	BUTYLENE	PENTANE	PENTYLENE	HEXANE	HEXYLENE	HEPTANE	HEPTYLENE	OCTANE	OCTYLENE	NONANE	NONYLENE	DECANE	DECYLENE	UNDECANE	UNDECYLENE	DODECANE	DODECYLENE	TRIDECANE	TRIDECYLENE	TETRADECANE	TETRADECYLENE	PENTADECANE	PENTADECYLENE	HEXADECANE	HEXADECYLENE	HEPTADECANE	HEPTADECYLENE	OCTADECANE	OCTADECYLENE	NONADECANE	NONADECYLENE	ICOSADECANE	ICOSADECYLENE	TRICOSADECANE	TRICOSADECYLENE	TETRACOSADECANE	TETRACOSADECYLENE	PENTACOSADECANE	PENTACOSADECYLENE	HEXACOSADECANE	HEXACOSADECYLENE	HEPTACOSADECANE	HEPTACOSADECYLENE	OCTACOSADECANE	OCTACOSADECYLENE	NONACOSADECANE	NONACOSADECYLENE	DECADECANE	DECADECYLENE	UNDECACANE	UNDECACYLENE	DODECACANE	DODECACYLENE	TRIDECACANE	TRIDECACYLENE	TETRADECACANE	TETRADECACYLENE	PENTADECACANE	PENTADECACYLENE	HEXADECACANE	HEXADECACYLENE	HEPTADECACANE	HEPTADECACYLENE	OCTADECACANE	OCTADECACYLENE	NONADECACANE	NONADECACYLENE	ICOSADECACANE	ICOSADECACYLENE	TRICOSADECACANE	TRICOSADECACYLENE	TETRACOSADECACANE	TETRACOSADECACYLENE	PENTACOSADECACANE	PENTACOSADECACYLENE	HEXACOSADECACANE	HEXACOSADECACYLENE	HEPTACOSADECACANE	HEPTACOSADECACYLENE	OCTACOSADECACANE	OCTACOSADECACYLENE	NONACOSADECACANE	NONACOSADECACYLENE	DECADECACANE	DECADECACYLENE	UNDECACACANE	UNDECACACYLENE	DODECACACANE	DODECACACYLENE	TRIDECACACANE	TRIDECACACYLENE	TETRADECACACANE	TETRADECACACYLENE	PENTADECACACANE	PENTADECACACYLENE	HEXADECACACANE	HEXADECACACYLENE	HEPTADECACACANE	HEPTADECACACYLENE	OCTADECACACANE	OCTADECACACYLENE	NONADECACACANE	NONADECACACYLENE	ICOSADECACACANE	ICOSADECACACYLENE	TRICOSADECACACANE	TRICOSADECACACYLENE	TETRACOSADECACACANE	TETRACOSADECACACYLENE	PENTACOSADECACACANE	PENTACOSADECACACYLENE	HEXACOSADECACACANE	HEXACOSADECACACYLENE	HEPTACOSADECACACANE	HEPTACOSADECACACYLENE	OCTACOSADECACACANE	OCTACOSADECACACYLENE	NONACOSADECACACANE	NONACOSADECACACYLENE	DECADECACACANE
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RUN NO = 77 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.060226	0.002004	0.009468	0.011033
2	1.624380	0.054073	0.255362	0.297591
3	30.040496	1.000000	4.722557	5.503505
4	1.953944	0.065043	0.307172	0.357968
5	0.840775	0.027988	0.132175	0.154032
6	0.880711	0.029317	0.138453	0.161348
7	0.267069	0.008890	0.041985	0.048927
8	0.055879	0.001860	0.008784	0.010237
9	1.076191	0.035824	0.169184	0.197161
10	0.043310	0.001441	0.006808	0.007934
11	0.341674	0.011373	0.053713	0.062595
12	1.398424	0.046551	0.219841	0.256195
13	53.413948	1.778064	8.397010	9.785589
14	0.035552	0.001183	0.005589	0.006513
15	0.018833	0.000626	0.002960	0.003450
16	0.508668	0.016932	0.079965	0.093189
17	2.935661	0.097723	0.461504	0.537821
18	0.171170	0.005697	0.026909	0.031358
19	2.821086	0.093909	0.443492	0.516831
20	0.672035	0.022370	0.105648	0.123118
21	0.048303	0.001607	0.007593	0.008849
22	0.015727	0.000523	0.002472	0.002881
23	0.066988	0.002229	0.010530	0.012272
24	0.190057	0.006326	0.029878	0.034819
25	0.071886	0.002392	0.011300	0.013169
26	0.027847	0.000927	0.004377	0.005101
27	0.038331	0.001276	0.006026	0.007022
28	0.021372	0.000711	0.003359	0.003915
29	0.353645	0.011772	0.055595	0.064788
30	0.005986	0.000199	0.000941	0.001096

TOTALS	099.999999	100.000030	3.328840
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CARBON BALANCE	7.898208 LB AT/MOLN2.	100.75 PERCENT
HYDROGEN BALANCE	19.689365 LB AT/MOLN2.	100.46 PERCENT
OXYGEN BALANCE	0.454723 LB AT/MOLN2.	85.53 PERCENT

PERCENT O2 REACT	79.6582	PERCENT C4 REACT	9.2716
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3579	0.0931	0.3187	0.2242	0.5955	0.1963	0.8252	0.5378
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.1228	0.2923	1.0000	0.7033	1.8682	0.6158	2.5886	1.6870
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2603	0.8905	0.6263	1.6637	0.5484	2.3053	1.5024
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.2185	0.5775	1.9757	1.3897	3.6911	1.2167	5.1145	3.3332

DATE: 10/10/2010 TIME: 10:10:10

ITEM NO.	ITEM NAME	QTY	UNIT	PRICE	TOTAL
1
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TOTAL 100.00000 100.00000 100.00000

OXYGEN BALANCE 0.00000 CARBON BALANCE 0.00000
HYDROGEN BALANCE 0.00000 NITROGEN BALANCE 0.00000
SULFUR BALANCE 0.00000 CHLORINE BALANCE 0.00000

PERCENT OF TOTAL 0.00000 PERCENT OF TOTAL 0.00000

ITEM NO.	ITEM NAME	QTY	UNIT	PRICE	TOTAL
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RUN NO = 77 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.303068	0.010071	0.040560	0.038784
2	0.527292	0.017522	0.070568	0.067479
3	30.092658	1.000000	4.027379	3.851037
4	2.625919	0.087261	0.351433	0.336045
5	1.523777	0.050636	0.203931	0.195001
6	1.351357	0.044906	0.180855	0.172936
7	0.481117	0.015987	0.064389	0.061569
8	0.124086	0.004123	0.016606	0.015879
9	0.740390	0.024603	0.099088	0.094749
10	0.042662	0.001417	0.005709	0.005459
11	0.326106	0.010836	0.043643	0.041732
12	1.596063	0.053038	0.213605	0.204252
13	51.160430	1.700096	6.846933	6.547137
14	0.028921	0.000961	0.003870	0.003701
15	0.018972	0.000630	0.002539	0.002427
16	0.531432	0.017659	0.071123	0.068008
17	4.071214	0.135289	0.544861	0.521004
18	0.166707	0.005539	0.022310	0.021333
19	2.753183	0.091490	0.368465	0.352332
20	0.764734	0.025412	0.102346	0.097865
21	0.064096	0.002129	0.008578	0.008202
22	0.023936	0.000795	0.003203	0.003063
23	0.064407	0.002140	0.008619	0.008242
24	0.131187	0.004359	0.017557	0.016788
25	0.096174	0.003195	0.012871	0.012307
26	0.060402	0.002007	0.008083	0.007729
27	0.037018	0.001230	0.004954	0.004737
28	0.000000	0.000000	0.000000	0.000000
29	0.292803	0.009730	0.039186	0.037470
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999938	099.999999	3.323069
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CARBON BALANCE	7.664731 LB AT/MOLN2.	97.77 PERCENT
HYDROGEN BALANCE	19.168750 LB AT/MOLN2.	97.81 PERCENT
OXYGEN BALANCE	0.440945 LB AT/MOLN2.	82.93 PERCENT

PERCENT O2 REACT	93.4082	PERCENT C4 REACT	13.2500
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.3360	0.0680	0.2459	0.3112	0.4057	0.1407	0.5700	0.5210
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.3661	0.2764	1.0000	1.2652	1.6494	0.5720	2.3175	2.1180
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2023	0.7319	0.9261	1.2073	0.4187	1.6964	1.5503
	MOLE	PRODUCT	PER MOLE	ETHENE			
1.9431	0.3932	1.4223	1.7997	2.3461	0.8137	3.2964	3.0126

RUN NO = 80

REACTOR ENTRANCE CONDITIONS

AIR = 3.20 LB/HR

BUTANE = 9.20 LB/HR

TEMPERATURE = 625.00 DEG F

PRESSURE = 53.50 LB/SQ IN

OXYGEN = 8.6517 NITROGEN = 32.5469 BUTANE = 58.8013 MOL PCNT

OXY/N = 0.2658 NIT/N = 1.0000 BUT/N = 1.8066 MOLS/MN2

BUTANE TO OXYGEN MOLAR RATIO = 6.7964

DENSITY OF GAS MIXTURE = 0.2116 LB/CU FT

GAS VELOCITY = 7.63 FT/SEC

RESIDENCE TIME BASED ON ENTRANCE CONDITIONS = 1.26 SEC

REYNOLDS NUMBER = 6412

1000 = 1000

REACTION RATE COEFFICIENT

AIR = 1.25 L/min 1000 = 1000

TEMPERATURE = 1000 = 1000

PRESSURE = 1000 = 1000

WEIGHT = 1000 = 1000

WEIGHT = 1000 = 1000

WEIGHT = 1000 = 1000

WEIGHT = 1000 = 1000

WEIGHT = 1000 = 1000

WEIGHT = 1000 = 1000

WEIGHT = 1000 = 1000

RUN NO = 80 SAMPLE NO = 1

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.000000	0.000000	0.000000	0.000000
2	5.578352	0.172038	1.834405	2.241549
3	32.425033	1.000000	10.662765	13.029350
4	0.299308	0.009230	0.098425	0.120270
5	0.075772	0.002336	0.024917	0.030447
6	0.026229	0.000808	0.008625	0.010539
7	0.001600	0.000049	0.000526	0.000642
8	0.000000	0.000000	0.000000	0.000000
9	1.258252	0.038804	0.413768	0.505603
10	0.162634	0.005015	0.053481	0.065351
11	0.323258	0.009969	0.106301	0.129895
12	0.450027	0.013879	0.147988	0.180834
13	56.092391	1.729910	18.445629	22.539604
14	0.000000	0.000000	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000
16	2.312039	0.071304	0.760299	0.929046
17	0.085737	0.002644	0.028194	0.034452
18	0.075571	0.002330	0.024851	0.030366
19	0.154333	0.004759	0.050751	0.062015
20	0.351409	0.010837	0.115558	0.141206
21	0.000000	0.000000	0.000000	0.000000
22	0.328119	0.010119	0.107900	0.131848
23	0.000000	0.000000	0.000000	0.000000
24	0.000000	0.000000	0.000000	0.000000
25	0.000000	0.000000	0.000000	0.000000
26	0.000000	0.000000	0.000000	0.000000
27	0.000000	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000	0.000000
29	0.000000	0.000000	0.000000	0.000000
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999969	99.999954	3.084036
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CARBON BALANCE	7.285101 LB AT/MOLN2.	100.80 PERCENT
HYDROGEN BALANCE	17.898559 LB AT/MOLN2.	99.06 PERCENT
OXYGEN BALANCE	0.526607 LB AT/MOLN2.	99.05 PERCENT

PERCENT O2 REACT	35.2807	PERCENT C4 REACT	4.2481
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.1202	0.9290	0.3107	0.0310	0.0620	0.1715	0.3654	0.0344
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
0.3870	2.9898	1.0000	0.1000	0.1995	0.5521	1.1760	0.1108
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	7.7246	2.5835	0.2585	0.5156	1.4265	3.0384	0.2864
	MOLE	PRODUCT	PER MOLE	ETHENE			
11.4113	88.1481	29.4820	2.9498	5.8840	16.2789	34.6728	3.2688

RUN NO = 80 SAMPLE NO = 2

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	1.251537	0.040573	0.186835	0.213007
2	1.500915	0.048658	0.224063	0.255451
3	30.845878	1.000000	4.604810	5.249876
4	2.758574	0.089430	0.411812	0.469501
5	0.773106	0.025063	0.115412	0.131580
6	0.940264	0.030482	0.140366	0.160030
7	0.174041	0.005642	0.025981	0.029621
8	0.000000	0.000000	0.000000	0.000000
9	1.377064	0.044643	0.205574	0.234372
10	0.085617	0.002775	0.012781	0.014571
11	0.403025	0.013065	0.060165	0.068593
12	1.661863	0.053876	0.248090	0.282844
13	49.852470	1.616179	7.442198	8.484741
14	0.004537	0.000147	0.000677	0.000772
15	0.005492	0.000178	0.000819	0.000934
16	1.081304	0.035055	0.161421	0.184034
17	3.068700	0.099484	0.458109	0.522283
18	0.169463	0.005493	0.025298	0.028842
19	2.062552	0.066866	0.307906	0.351040
20	0.908468	0.029451	0.135620	0.154618
21	0.000000	0.000000	0.000000	0.000000
22	0.488200	0.015827	0.072880	0.083090
23	0.062975	0.002041	0.009401	0.010718
24	0.147433	0.004779	0.022009	0.025092
25	0.063624	0.002062	0.009498	0.010828
26	0.011507	0.000373	0.001717	0.001958
27	0.012480	0.000404	0.001863	0.002124
28	0.000000	0.000000	0.000000	0.000000
29	0.289041	0.009370	0.043149	0.049193
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999954	99.999984	3.241924
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CARBON	BALANCE	7.330579 LB AT/MOLN2.	101.43 PERCENT
HYDROGEN	BALANCE	18.145484 LB AT/MOLN2.	100.43 PERCENT
OXYGEN	BALANCE	0.493014 LB AT/MOLN2.	92.73 PERCENT

PERCENT O2 REACT	81.6951	PERCENT C4 REACT	10.5432
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.4695	0.1840	0.3514	0.3742	0.4021	0.2106	0.7175	0.5222
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.3359	0.5236	1.0000	1.0647	1.1444	0.5994	2.0416	1.4861
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.3919	0.7485	0.7970	0.8566	0.4487	1.5282	1.1124
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.9338	1.1499	2.1960	2.3383	2.5132	1.3164	4.4835	3.2636

Report of the Board of Directors for the year ended December 31, 1999

Item	1999	1998	1997	1996	1995
1. Cash and cash equivalents	1,234,567	1,123,456	1,012,345	901,234	890,123
2. Accounts receivable	2,345,678	2,234,567	2,123,456	2,012,345	1,901,234
3. Inventory	3,456,789	3,345,678	3,234,567	3,123,456	3,012,345
4. Prepaid expenses	4,567,890	4,456,789	4,345,678	4,234,567	4,123,456
5. Other assets	5,678,901	5,567,890	5,456,789	5,345,678	5,234,567
6. Total assets	17,283,825	16,728,320	16,172,815	15,617,316	15,161,815
7. Accounts payable	1,234,567	1,123,456	1,012,345	901,234	890,123
8. Long-term debt	2,345,678	2,234,567	2,123,456	2,012,345	1,901,234
9. Other liabilities	3,456,789	3,345,678	3,234,567	3,123,456	3,012,345
10. Total liabilities	7,037,034	6,703,701	6,370,368	6,037,035	5,803,702
11. Total equity	10,246,791	10,024,619	9,802,447	9,580,281	9,358,113

Item	1999	1998	1997	1996	1995
1. Cash and cash equivalents	1,234,567	1,123,456	1,012,345	901,234	890,123
2. Accounts receivable	2,345,678	2,234,567	2,123,456	2,012,345	1,901,234
3. Inventory	3,456,789	3,345,678	3,234,567	3,123,456	3,012,345
4. Prepaid expenses	4,567,890	4,456,789	4,345,678	4,234,567	4,123,456
5. Other assets	5,678,901	5,567,890	5,456,789	5,345,678	5,234,567
6. Total assets	17,283,825	16,728,320	16,172,815	15,617,316	15,161,815
7. Accounts payable	1,234,567	1,123,456	1,012,345	901,234	890,123
8. Long-term debt	2,345,678	2,234,567	2,123,456	2,012,345	1,901,234
9. Other liabilities	3,456,789	3,345,678	3,234,567	3,123,456	3,012,345
10. Total liabilities	7,037,034	6,703,701	6,370,368	6,037,035	5,803,702
11. Total equity	10,246,791	10,024,619	9,802,447	9,580,281	9,358,113

RUN NO = 80 SAMPLE NO = 3

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	1.279242	0.040573	0.161284	0.160842
2	0.449476	0.014256	0.056669	0.056513
3	31.528709	1.000000	3.975090	3.964198
4	3.268219	0.103658	0.412051	0.410922
5	0.810691	0.025712	0.102210	0.101930
6	1.117298	0.035437	0.140867	0.140481
7	0.234770	0.007446	0.029599	0.029518
8	0.000000	0.000000	0.000000	0.000000
9	1.284831	0.040751	0.161989	0.161545
10	0.054147	0.001717	0.006826	0.006808
11	0.410127	0.013008	0.051708	0.051566
12	2.047757	0.064948	0.258177	0.257470
13	49.008300	1.554402	6.178888	6.161958
14	0.012115	0.000384	0.001527	0.001523
15	0.009312	0.000295	0.001174	0.001170
16	0.680772	0.021592	0.085830	0.085595
17	3.588767	0.113825	0.452466	0.451226
18	0.121281	0.003846	0.015290	0.015249
19	2.232441	0.070806	0.281462	0.280691
20	0.809787	0.025684	0.102096	0.101816
21	0.000000	0.000000	0.000000	0.000000
22	0.513560	0.016288	0.064748	0.064571
23	0.047278	0.001499	0.005960	0.005944
24	0.135634	0.004301	0.017100	0.017053
25	0.048329	0.001532	0.006093	0.006076
26	0.020217	0.000641	0.002549	0.002542
27	0.019891	0.000630	0.002507	0.002501
28	0.056091	0.001779	0.007071	0.007052
29	0.211103	0.006695	0.026615	0.026542
30	0.000000	0.000000	0.000000	0.000000

TOTALS	99.999938	100.000030	3.171712
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CARBON BALANCE	7.119027 LB AT/MOLN2.	98.51 PERCENT
HYDROGEN BALANCE	17.634323 LB AT/MOLN2.	97.60 PERCENT
OXYGEN BALANCE	0.422887 LB AT/MOLN2.	79.54 PERCENT

PERCENT O2 REACT	94.6369	PERCENT C4 REACT	13.9626
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.4109	0.0855	0.3090	0.2922	0.3097	0.1366	0.5300	0.4512
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.3296	0.2769	1.0000	0.9458	1.0023	0.4420	1.7151	1.4601
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.2083	0.7520	0.7113	0.7538	0.3324	1.2898	1.0980
	MOLE	PRODUCT	PER MOLE	ETHENE			
2.9251	0.6093	2.1998	2.0806	2.2051	0.9725	3.7730	3.2120

RUN NO = 80 SAMPLE NO = 4

PRD NO	MOL PERCENT	MOLS/MOL N2	MOLS/MOXY R	MOLS/MBUT R
1	0.490970	0.015562	0.061753	0.060507
2	0.435583	0.013807	0.054786	0.053681
3	31.547794	1.000000	3.968007	3.887963
4	3.477710	0.110236	0.437418	0.428594
5	0.874992	0.027735	0.110054	0.107834
6	1.119781	0.035494	0.140843	0.138002
7	0.258821	0.008204	0.032553	0.031897
8	0.000000	0.000000	0.000000	0.000000
9	1.658715	0.052577	0.208629	0.204420
10	0.092682	0.002937	0.011657	0.011422
11	0.585884	0.018571	0.073691	0.072204
12	1.906960	0.060446	0.239852	0.235014
13	48.881919	1.549456	6.148253	6.024228
14	0.009952	0.000315	0.001251	0.001226
15	0.011428	0.000362	0.001437	0.001408
16	0.516662	0.016377	0.064984	0.063673
17	3.774159	0.119633	0.474704	0.465129
18	0.174567	0.005533	0.021956	0.021513
19	2.310658	0.073243	0.290629	0.284766
20	0.755790	0.023956	0.095061	0.093143
21	0.000000	0.000000	0.000000	0.000000
22	0.529407	0.016781	0.066587	0.065244
23	0.049999	0.001584	0.006288	0.006161
24	0.145623	0.004615	0.018316	0.017946
25	0.074374	0.002357	0.009354	0.009165
26	0.005476	0.000173	0.000688	0.000674
27	0.018285	0.000579	0.002299	0.002253
28	0.060940	0.001931	0.007664	0.007510
29	0.231019	0.007322	0.029057	0.028470
30	0.000000	0.000000	0.000000	0.000000
TOTALS	99.999938	100.000030	3.169794	

CARBON BALANCE	7.155912 LB AT/MOLN2.	99.02 PERCENT
HYDROGEN BALANCE	17.670410 LB AT/MOLN2.	97.80 PERCENT
OXYGEN BALANCE	0.428318 LB AT/MOLN2.	80.56 PERCENT

PERCENT O2 REACT	94.8059	PERCENT C4 REACT	14.2364
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CO	CO2	BUTEN	PARFIN	ALCOHL	ALDHYD	OXYGCO	WATER
	MOLE	PRODUCT	PER MOLE	N-BUTANE			
0.4285	0.0636	0.3072	0.2002	0.3139	0.1348	0.5368	0.4651
	MOLE	PRODUCT	PER MOLE	N-BUTENES			
1.3950	0.2072	1.0000	0.6517	1.0217	0.4389	1.7474	1.5139
	MOLE	PRODUCT	PER MOLE	CO			
1.0000	0.1485	0.7168	0.4671	0.7324	0.3146	1.2525	1.0852
	MOLE	PRODUCT	PER MOLE	ETHENE			
3.1057	0.4613	2.2261	1.4509	2.2746	0.9772	3.8901	3.3704

PERCENT OF SECT	2000-01	2001-02	2002-03	2003-04	2004-05	2005-06	2006-07	2007-08	2008-09	2009-10	2010-11	2011-12	2012-13	2013-14	2014-15	2015-16	2016-17	2017-18	2018-19	2019-20	2020-21	2021-22	2022-23	2023-24	2024-25	2025-26	2026-27	2027-28	2028-29	2029-30	2030-31	2031-32	2032-33	2033-34	2034-35	2035-36	2036-37	2037-38	2038-39	2039-40	2040-41	2041-42	2042-43	2043-44	2044-45	2045-46	2046-47	2047-48	2048-49	2049-50	2050-51	2051-52	2052-53	2053-54	2054-55	2055-56	2056-57	2057-58	2058-59	2059-60	2060-61	2061-62	2062-63	2063-64	2064-65	2065-66	2066-67	2067-68	2068-69	2069-70	2070-71	2071-72	2072-73	2073-74	2074-75	2075-76	2076-77	2077-78	2078-79	2079-80	2080-81	2081-82	2082-83	2083-84	2084-85	2085-86	2086-87	2087-88	2088-89	2089-90	2090-91	2091-92	2092-93	2093-94	2094-95	2095-96	2096-97	2097-98	2098-99	2099-00	2100-01	2101-02	2102-03	2103-04	2104-05	2105-06	2106-07	2107-08	2108-09	2109-10	2110-11	2111-12	2112-13	2113-14	2114-15	2115-16	2116-17	2117-18	2118-19	2119-20	2120-21	2121-22	2122-23	2123-24	2124-25	2125-26	2126-27	2127-28	2128-29	2129-30	2130-31	2131-32	2132-33	2133-34	2134-35	2135-36	2136-37	2137-38	2138-39	2139-40	2140-41	2141-42	2142-43	2143-44	2144-45	2145-46	2146-47	2147-48	2148-49	2149-50	2150-51	2151-52	2152-53	2153-54	2154-55	2155-56	2156-57	2157-58	2158-59	2159-60	2160-61	2161-62	2162-63	2163-64	2164-65	2165-66	2166-67	2167-68	2168-69	2169-70	2170-71	2171-72	2172-73	2173-74	2174-75	2175-76	2176-77	2177-78	2178-79	2179-80	2180-81	2181-82	2182-83	2183-84	2184-85	2185-86	2186-87	2187-88	2188-89	2189-90	2190-91	2191-92	2192-93	2193-94	2194-95	2195-96	2196-97	2197-98	2198-99	2199-00	2200-01	2201-02	2202-03	2203-04	2204-05	2205-06	2206-07	2207-08	2208-09	2209-10	2210-11	2211-12	2212-13	2213-14	2214-15	2215-16	2216-17	2217-18	2218-19	2219-20	2220-21	2221-22	2222-23	2223-24	2224-25	2225-26	2226-27	2227-28	2228-29	2229-30	2230-31	2231-32	2232-33	2233-34	2234-35	2235-36	2236-37	2237-38	2238-39	2239-40	2240-41	2241-42	2242-43	2243-44	2244-45	2245-46	2246-47	2247-48	2248-49	2249-50	2250-51	2251-52	2252-53	2253-54	2254-55	2255-56	2256-57	2257-58	2258-59	2259-60	2260-61	2261-62	2262-63	2263-64	2264-65	2265-66	2266-67	2267-68	2268-69	2269-70	2270-71	2271-72	2272-73	2273-74	2274-75	2275-76	2276-77	2277-78	2278-79	2279-80	2280-81	2281-82	2282-83	2283-84	2284-85	2285-86	2286-87	2287-88	2288-89	2289-90	2290-91	2291-92	2292-93	2293-94	2294-95	2295-96	2296-97	2297-98	2298-99	2299-00	2300-01	2301-02	2302-03	2303-04	2304-05	2305-06	2306-07	2307-08	2308-09	2309-10	2310-11	2311-12	2312-13	23																																																																																																																																																																																																																																																																																																																																																																																			
OTHER BALANCE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	

APPENDIX F

Transported Bed Reactor Model

Model Description

Parameter	Value	Unit
μ_{max}	0.8	1/d
K_s	0.1	g/L
$Y_{x/s}$	0.5	g/g
$Y_{p/s}$	0.2	g/g
$Y_{p/x}$	0.4	g/g
m	0.05	1/d
k_d	0.01	1/d

Model Equations

Mass Balance Equations

Substrate Balance

APPENDIX F

TRANSPORTED BED REACTOR MODEL

Model Description

Mass Balance Equations

Substrate Balance

Cell Balance

Product Balance

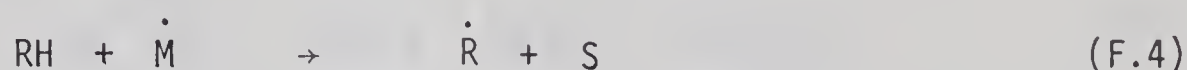
Parameter Values

Model Equations

Model Results

Derivation of the Rate Equations

The following reaction scheme was used for the preliminary evaluation of the TBR.



where RH stands for the hydrocarbon, \dot{M} for free radical, \dot{R} for alkyl radical, P for an intermediate and Q and S for end products.

Solution of these equations, using the method of quasi-stationary state in chain reaction mechanism leads to

$$C_{A_0} \frac{dx_A}{dt} = K_1 C_{A_0} C_{B_0} (1 - x_A)(1 - x_B) \{1 + 2C_{A_0} K_3 (1 - x_A)\} \\ + C_{A_0}^2 C_{B_0} K_2 K_3 (1 - x_A)(1 - x_B) x_C \quad (F.6)$$

$$= K_1 C_1 (1 + 2K_3 C_7) + K_2 K_3 C_{A_0} C_1 x_C \quad (F.7)$$

$$\text{where } C_1 = C_{A_0} C_{B_0} (1 - x_A)(1 - x_B)$$

$$C_2 = C_{A_0} C_{B_0} (1 - x_B) x_C$$

$$C_7 = C_{A_0} (1 - x_A) \quad \text{and}$$

C_{A_0} and C_{B_0} are the initial concentrations of n-butane and oxygen, respectively, x_A and x_B their conversions, and x_C the accumulation of

the intermediate species P expressed as

$$x_C = \frac{C_C}{C_{A_0}}$$

where C_C is the concentration of the species P.

The rate constant K_3 above is in fact the ratio of rate constants for reactions (4) and (5).

The other two rate equations are:

$$C_{B_0} \frac{dx_B}{dt} = (2K_1C_1 + K_2C_2)(1 + K_3C_{A_0}C_7) \quad (F.8)$$

$$C_{A_0} \frac{dx_C}{dt} = K_1C_1(1 + 2K_3C_7) + K_2C_2(K_3C_7C_{A_0} - 1) \quad (F.9)$$

An overall heat of reaction is used and is combined with the conversion equation for oxygen as the heat generation term in equation 7.3.

Derivation of the Heat Conduction Equation

Assumptions:

1. Solids temperature symmetrical.
2. Thermal conductivity and specific heat of solids are constant.
3. Neglect all second order or higher differentials (dr).

Consider as in figure F.1 a heat balance about a spherical shell of radius r and thickness dr .

$$\text{Heat in} = -4\pi r^2 K_s \left(\frac{\partial v}{\partial r} \right) dt$$

$$\text{Heat out} = -4\pi (r + dr)^2 K_s \left(\frac{\partial v}{\partial r} + \frac{\partial}{\partial r} \frac{\partial v}{\partial r} dr \right) dt$$

$$\text{Accumulation} = \rho_s c_s \frac{4}{3}\pi [(r + dr)^3 - r^3] dv$$

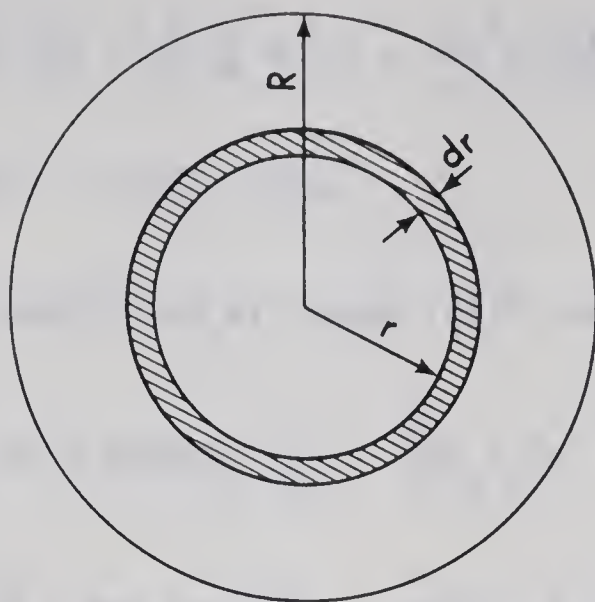


FIGURE F.1 HEAT BALANCE FOR A SPHERICAL PARTICLE

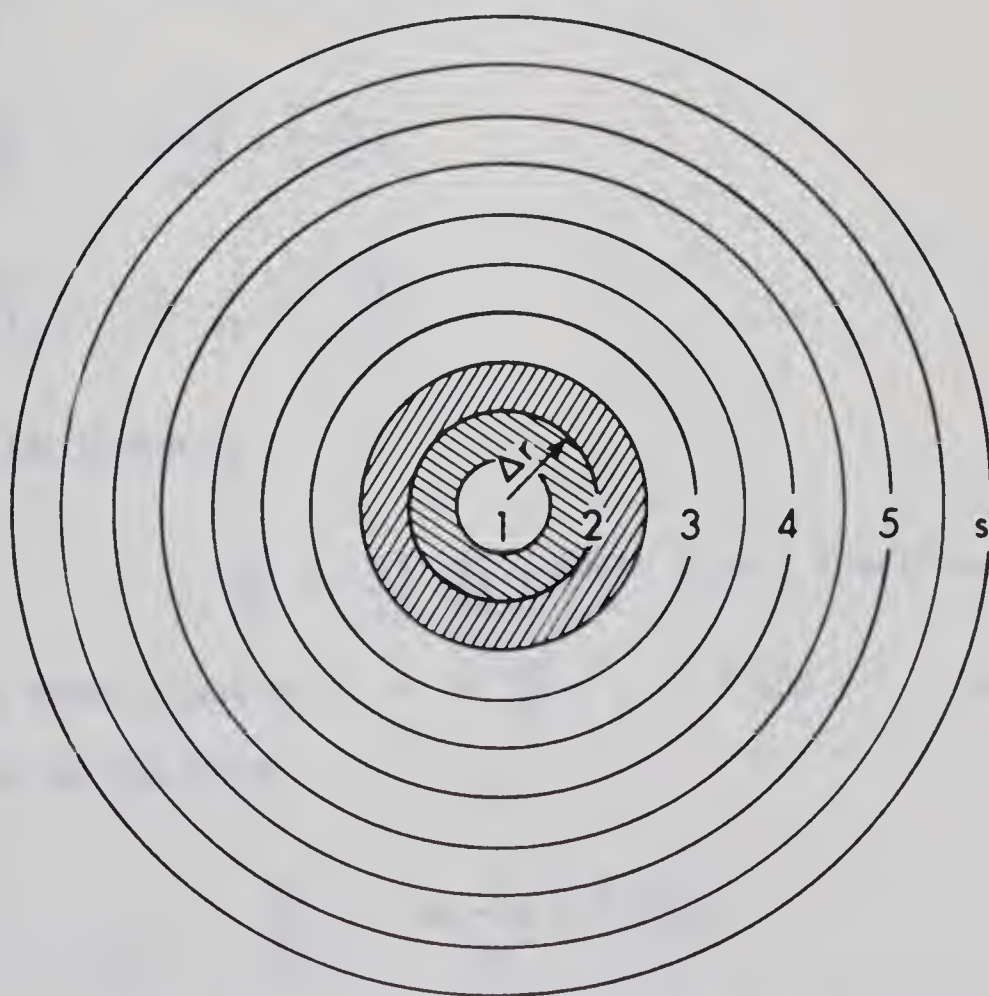


FIGURE F.2 DISCRETISATION OF THE SPHERICAL SHELL

$$\begin{aligned} \therefore 4\pi(r + dr)^2 K_s \left(\frac{\partial v}{\partial r} + \frac{\partial}{\partial r} \frac{\partial v}{\partial r} dr \right) dt - 4\pi r^2 K_s \left(\frac{\partial v}{\partial r} \right) dt \\ = \rho_s C_s \frac{4}{3} \pi [(r + dr)^3 - r^3] dv \end{aligned}$$

Multiplying and neglecting all terms $(dr)^2$ and higher

$$4\pi r^2 K_s \frac{\partial^2 v}{\partial r^2} dr + 8\pi r dr K_s \frac{\partial v}{\partial r} = \frac{4}{3} \pi \rho_s C_s (r^3 + 3r^3 dr - r^3) \frac{\partial v}{\partial t}$$

$$\therefore 4\pi r^2 K_s \frac{\partial^2 v}{\partial r^2} + 8\pi r dr K_s \frac{\partial v}{\partial r} = 4\pi^2 dr \rho_s C_s \frac{\partial v}{\partial t}$$

$$\therefore \frac{K_s}{\rho_s C_s} \left(\frac{\partial^2 v}{\partial r^2} + \frac{2}{r} \frac{\partial v}{\partial r} \right) = \frac{\partial v}{\partial t}$$

But $\frac{K_s}{\rho_s C_s} = \alpha$, the thermal diffusivity

$$\therefore \frac{\partial v}{\partial t} = \alpha \left(\frac{\partial^2 v}{\partial r^2} + \frac{2}{r} \frac{\partial v}{\partial r} \right) \quad (F.10)$$

$$\text{or, } \frac{\partial v}{\partial t} = \frac{\alpha}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial v}{\partial r} \right) \quad (F.11)$$

Using the property

$$\frac{\partial f}{\partial \eta} = \frac{\partial f}{\partial \xi} \frac{d\xi}{d\eta}, \text{ where } \xi \text{ is a function of } \eta \text{ only,}$$

in the above equation $f = r^2 \frac{\partial v}{\partial r}$, $\xi = r^3$ and $\eta = r$, equation (F.11)

reduces to the form

$$\frac{\partial v}{\partial t} = 3\alpha \frac{\partial}{\partial r^3} \left(r^2 \frac{\partial v}{\partial r} \right) \quad (F.12)$$

This equation is reduced to a convenient form by discretizing the space derivative while treating the time derivative as a continuous derivative.

Discretisation of the Heat Conduction Equation

For a sphere divided into five equal segments as in figure (F.2), the discretisation of the space variable in equation (F.12) gives, for point 1,

$$\begin{aligned}
 \frac{dv_1}{dt} &= 3\alpha \left[\frac{\left(\frac{r_2 + r_1}{2}\right)^2 \left(\frac{v_2 - v_1}{r_2 - r_1}\right)}{\left(\frac{r_2 + r_1}{2}\right)^3} \right] \\
 &= 3\alpha \frac{\Delta r}{4} \frac{-v_1 + v_2}{\frac{\Delta r^3}{8}} \\
 &= \frac{6\alpha}{\Delta r^2} (-v_1 + v_2)
 \end{aligned}$$

$$\text{or, } \frac{1}{6} \frac{dv_1}{dt} = \frac{\alpha}{\Delta r^2} (-v_1 + v_2) \quad (\text{F.13})$$

For point 2,

$$\begin{aligned}
 \frac{dv_2}{dt} &= 3\alpha \frac{\left(\frac{r_3 + r_2}{2}\right)^2 \left(\frac{v_3 - v_2}{r_3 - r_2}\right) - \left(\frac{r_2 + r_1}{2}\right)^2 \left(\frac{v_2 - v_1}{r_2 - r_1}\right)}{\left(\frac{r_2 + r_3}{2}\right)^3 - \left(\frac{r_2 + r_1}{2}\right)^3} \\
 &= 3\alpha \frac{\Delta r}{4} \frac{9(v_3 - v_2) - (v_2 - v_1)}{\Delta r^3 \left(\frac{27}{8} - \frac{1}{8}\right)} \\
 &= \frac{3}{13} \frac{\alpha}{\Delta r^2} (v_1 - 10v_2 + 9v_3)
 \end{aligned}$$

$$\text{or, } \frac{13}{3} \frac{dv_2}{dt} = \frac{\alpha}{\Delta r^2} (v_1 - 10v_2 + 9v_3) \quad (\text{F.14})$$

For point 3,

$$\frac{dv_3}{dt} = 3\alpha \frac{\left(\frac{r_4 + r_3}{2}\right)^2 \left(\frac{v_4 - v_3}{r_4 - r_3}\right) - \left(\frac{r_3 + r_2}{2}\right)^2 \left(\frac{v_3 - v_2}{r_3 - r_2}\right)}{\left(\frac{r_4 + r_3}{2}\right)^3 - \left(\frac{r_3 + r_2}{2}\right)^3}$$

$$\text{or, } \frac{49}{3} \frac{dv_3}{dt} = \frac{\alpha}{\Delta r^2} (9v_2 - 34v_3 + 25v_4) \quad (\text{F.15})$$

For point 4,

$$\frac{dv_4}{dt} = 3\alpha \frac{\left(\frac{r_5 + r_4}{2}\right)^2 \left(\frac{v_5 - v_4}{r_5 - r_4}\right) - \left(\frac{r_4 + r_3}{2}\right)^2 \left(\frac{v_4 - v_3}{r_4 - r_3}\right)}{\left(\frac{r_5 + r_4}{2}\right)^3 - \left(\frac{r_4 + r_3}{2}\right)^3}$$

$$\text{or, } \frac{109}{3} \frac{dv_4}{dt} = \frac{\alpha}{\Delta r^2} (25v_3 - 74v_4 + 49v_5) \quad (\text{F.16})$$

For point 5,

$$\frac{dv_5}{dt} = 3\alpha \frac{\left(\frac{r_5 + \Delta r + r_5}{2}\right)^2 \left(\frac{v_5 - v_5}{r_5 + \Delta r - r_5}\right) - \left(\frac{r_5 + r_4}{2}\right)^2 \left(\frac{v_5 - v_4}{r_5 - r_4}\right)}{\left(\frac{r_5 + \Delta r + r_5}{2}\right)^3 - \left(\frac{r_5 + r_4}{2}\right)^3}$$

$$\text{or, } \frac{193}{3} \frac{dv_5}{dt} = \frac{\alpha}{\Delta r^2} (49v_4 - 130v_5 + 81v_5) \quad (\text{F.17})$$

Equations (F.4) to (F.8) are now in the form

$$\underline{G} \frac{d\underline{y}}{dt} = \frac{\alpha}{\Delta r^2} (\underline{B} \underline{y} + \underline{S}'(t)) \quad (\text{F.18})$$

where

$$\underline{G} = \begin{bmatrix} 1/6 & 0 & 0 & 0 & 0 \\ 0 & 13/3 & 0 & 0 & 0 \\ 0 & 0 & 49/3 & 0 & 0 \\ 0 & 0 & 0 & 109/3 & 0 \\ 0 & 0 & 0 & 0 & 193/3 \end{bmatrix} \quad (\text{F.19})$$

$$\underline{B} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 1 & -10 & 9 & 0 & 0 \\ 0 & 9 & -34 & 25 & 0 \\ 0 & 0 & 25 & -74 & 49 \\ 0 & 0 & 0 & 49 & -130 \end{bmatrix} \quad (\text{F.20})$$

and

$$S'(t) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 81v_s \end{bmatrix} \quad (\text{F.21})$$

In order to make the solution independent of the properties of the solids and the diameter of the solid particles, the equation (F.18) is nondimensionalized.

Let

$$\theta = \frac{\alpha t}{\Delta r^2}$$

$$d\theta = \frac{\alpha}{\Delta r^2} dt$$

$$\therefore \underline{G} \frac{d\underline{y}}{d\theta} \frac{\alpha}{\Delta r^2} = \frac{\alpha}{\Delta r^2} [\underline{B} \underline{y} + \underline{S}(\theta)]$$

(F.22)

$$\underline{G} \frac{d\underline{y}}{d\theta} = \underline{B} \underline{y} + \underline{S}(\theta)$$

Method of Solution

The solution to this matrix differential equation has been obtained in a closed form as:

$$\underline{y}(\theta, r) = \underline{G}^{-1/2} \underline{Q} \underline{E}(\theta) \underline{Q}^T \underline{G}^{1/2} [\underline{y}^{(0)} + \int_0^\theta \underline{G}^{-1/2} \underline{Q} \underline{E}^{-1}(\sigma) \underline{Q}^T \underline{G}^{-1/2}$$

$$\underline{S}(\sigma) d\sigma]$$

(F.23)

A direct numerical solution to this leads to instability. A numerically suitable form can be obtained by simplification of the above. Multiplying out the terms, one obtains

$$\underline{y}(\theta, r) = \underline{G}^{-1/2} \underline{Q} \underline{E}(\theta) \underline{Q}^T \underline{G}^{1/2} \underline{y}^{(0)} + \underline{G}^{-1/2} \underline{Q} \underline{E}(\theta) \int_0^\theta \underline{E}^{-1}(\sigma) \underline{Q}^T \underline{G}^{-1/2} \underline{S}(\sigma) d\sigma$$

$$= \underline{G}^{-1/2} \underline{Q} [\underline{E}(\theta) \underline{Q}^T \underline{G}^{1/2} \underline{y}^{(0)} + \underline{E}(\theta) \int_0^\theta \underline{E}^{-1}(\sigma) \underline{Q}^T \underline{G}^{-1/2} \underline{S}(\sigma) d\sigma]$$

$$= \underline{D} [\underline{E}(\theta) \underline{y} \underline{y}^{(0)} + \underline{E}(\theta) \int_0^\theta \underline{E}^{-1}(\sigma) \underline{H} \underline{S}(\sigma) d\sigma]$$

(F.24)

where $\underline{D} = \underline{G}^{-1/2} \underline{Q}$, $\underline{V} = \underline{Q}^T \underline{G}^{1/2}$ and $\underline{H} = \underline{Q}^T \underline{G}^{-1/2}$.

If the boundary condition vector is of the form

$$\underline{S}(\theta) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \phi(\theta) \end{bmatrix},$$

the matrix \underline{H} can be replaced by a vector \underline{p} , which is the last column for the matrix \underline{H} . The second term in equation (F.15) is thus

$$\underline{E}(\theta) \int_0^\theta \underline{E}^{-1}(\sigma) \underline{p} \phi(\sigma) d\sigma \quad (\text{F.25})$$

Realizing that the matrices $\underline{E}(\theta)$ and $\underline{E}^{-1}(\sigma)$ are diagonal matrices, the above integration and the subsequent multiplication can be performed term by term. Considering the i th element, the above term is,

$$e^{\lambda_i \theta} \int_0^\theta e^{-\lambda_i \sigma} p_i \phi(\sigma) d\sigma \quad (\text{F.26})$$

The integral can be evaluated for any function $\phi(\sigma)$. If

$$\phi(\sigma) = a_0 + b\sigma, \quad (\text{F.27})$$

Integration by parts leads to

$$\begin{aligned}
& e^{\lambda_i \theta} \left[\left(\frac{a_0}{\lambda_i} + \frac{b}{\lambda_i^2} \right) (1 - e^{-\lambda_i \theta}) - \frac{b}{\lambda_i} \theta e^{-\lambda_i \theta} \right] v_i \\
& = v_i \left[\left(\frac{a_0}{\lambda_i} + \frac{b}{\lambda_i^2} \right) (e^{\lambda_i \theta} - 1) - \frac{b}{\lambda_i} \theta \right]
\end{aligned} \tag{F.28}$$

The first term in the parenthesis in equation (F.24) is obtained by post multiplying the matrix \underline{V} with the initial condition vector $\underline{v}^{(0)}$ and premultiplying the resultant vector with the matrix $\underline{E}(\theta)$.

The two parts of the solution are then combined and multiplied by matrix \underline{D} to obtain the temperatures.

The heat transfer from the gas to the solids is given by

$$Q_g = [(cT_2 + cT_1)G_g - h_w A_w (T - T_w) dZ + A_r dZ (-r\Delta H)] \theta \tag{F.29}$$

This must be equal to the heat received by the solids:

$$Q_s = h_c A_s dZ (T - v_s) \theta = A_s dZ \int_0^\theta K_s \left(\frac{\partial v}{\partial r} \right)_{r=R} d\theta \tag{F.30}$$

This can be more easily obtained by integrating over the whole surface of the solids.

$$Q_s = NdZ \int_0^R c_p \rho_p 4\pi r^2 (v^{(1)} - v^{(0)}) dr, \tag{F.31}$$

where $v^{(0)}$ and $v^{(1)}$ are the temperatures at the beginning and at the end of the increments respectively.

The algorithm is now as follows:

1. Assume $a_0 = v_s^{(0)}$, where $v_s^{(0)}$ is the initial condition or is known from the previous increment. Obtain $v_s^{(1)}$ by a heat balance at the

surface.

2. Obtain $b = \frac{v_s^{(1)} - a_0}{\theta}$
3. Solve the gas phase equations.
4. Obtain Q_g .
5. Solve the matrix differential equation for the solids phase.
6. Obtain Q_s .
7. If $|Q_g - Q_s| < \epsilon$, go to next increment and repeat.
8. If $|Q_g - Q_s| > \epsilon$, obtain a new b as follows:

$$Q = h_c A_s dZ (T - v_s), \text{ where}$$

$$Q = \frac{Q_s + Q_g}{2} \text{ and } v_s = a_0 + \frac{1}{2} b \theta$$

$$\therefore b = \frac{2}{\theta} \left(T - a_0 - \frac{Q}{h_c A_s dZ \theta} \right)$$

Perturb b if necessary.

9. Go to 3 and interate.

A value of 0.05 has been used in the calculations for λ which has been redefined as

$$\lambda = \frac{2|Q_g - Q_s|}{|Q_g + Q_s|}$$

The value of the perturbation factor for b depends on the diameter of the particle and is obtained by trial and error.

The computer program and some sample results are now presented.

C TBR

C TBR

C THIS PROGRAM SOLVES A COUPLED SYSTEM OF A SET OF
C ORDINARY DIFFERENTIAL EQUATIONS AND A PARABOLIC
C PARTIAL DIFFERENTIAL EQUATION. THE SYSTEM IS DECOU-
C PLED AND SOLVED SEPARATELY.
C THE STATE VARIABLES ARE NORMALISED SO THAT THEIR
C VALUES DO NOT EXCEED 12.0.
C THE PERTURBATION FACTOR IS OBTAINED BY TRIAL AND
C ERROR, USUALLY STARTING AT A LOWER VALUE AND
C SLOWLY INCREASING TO THE DESIRED VALUE.
C THE PROGRAM USES NINE SUBROUTINES INCLUDING THE
C FORS SUBROUTINE FOR WALL TEMPERATURE PROFILE.
C THE SUBROUTINES ARE PRESENTED FOLLOWED BY THE
C MAINLINE PROGRAM. THE PURPOSE OF EACH SUBROUTINE
C IS OUTLINED AT THE BEGINNING OF EACH SUBROUTINE.
C THE MAINLINE PROGRAM READS IN THE INITIAL CONDI-
C TIONS AND INPUT MATRICES, DIRECTS THE SOLUTION
C AND PRINTS OUT THE RESULTS.
C

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CAO,CBO
DIMENSION TY(8),D(8),QR(8),AA(8),EA(8),TT(12),R(12)
*,W(8)
DIMENSION T(200,12),S(8,4),U(12)
DIMENSION A(78),UO(12),TC2(12),TN(12)
DIMENSION B(12,12),V(12,12),G(12,12),TI(8)

C M NUMBER OF REACTION EQUATIONS 9
C N NUMBER OF RADIAL DIVISIONS 13
C MM NUMBER OF DIFFERENTIAL EQUATIONS 9
C MG NUMBER OF GAS FLOW RATES
C ML NUMBER OF LOADING RATIOS
C MR NUMBER OF PARTICLE DIAMETERS
C MT NUMBER OF PARTICLE MATERIALS
C N4 NUMBER OF INCREMENTS ALONG LENGTH OF REACTOR
C DIF TEMPERATURE DIFFERENCE BETWEEN GAS AND SOLIDS
C SURFACE
C DL LENGTH ALONG REACTOR
C ES ALLOWABLE ERROR IN BOUNDARY CONDITION MATCHING
C FL LENGTH OF REACTOR
C FT PERTURBATION FACTOR FOR MATCHING
C HR HEAT OF REACTION
C T TEMPERATURE OF SOLID PARTICLES
C TB BASE TEMPERATURE
C TG TEMPERATURE OF GAS
C TS SURFACE TEMPERATURE OF PARTICLES
C TW WALL TEMPERATURE OF REACTOR
C XA CONVERSION OF BUTANE

AND PRINTS OUT THE RESULTS.

THE MAINLINE PROGRAM READS IN THE INITIAL CONDITIONS AND INPUT MATRICES. IT SETS THE SOLUTION IS OBTAINED AT THE BEGINNING OF EACH SUBROUTINE. THE SUBROUTINES ARE LISTED FOLLOWED BY THE FOUR SUBROUTINE FOR ALL TEMPERATURE POINTS. THE PROGRAM USES THE SUBROUTINES TWICE FOR EACH POINT INCREASING TO THE DESIRED VALUE.

THE REFORMATION FACTOR IS OBTAINED BY TAKING THE VALUES OF THE FACTOR EXCEED 15.0.

THE STATE VARIABLES ARE NORMALIZED SO THAT THE VALUES ARE BETWEEN 0.0 AND 1.0.

THE PROGRAM SOLVES THE DIFFERENTIAL EQUATIONS BY USING THE RUNGE-KUTTA METHOD. THE RESULTS ARE PRINTED OUT AT THE END OF EACH SUBROUTINE.

DIMENSION 8 (S, S), V(I, I), S(I, I), R(I, I), T(I, I)
DIMENSION A(30), W(I, I), TC(S, I), TW(I, I)
DIMENSION T(500, I), Z(I, +), H(I, I)

4-NIB)
DIMENSION TY(R), Q(R), QR(I), RA(I), EA(D), J(I, I), L(I, I)
COMMON F1, F2, F3, F4, F5, F6, F7, F8, F9, G0, G1
COMMON A1, A2, A3, A4, E, T1, G2, G3, DRR, FR

[illegible]

C TBR ... (CONT'D)

C XB CONVERSION OF OXYGEN
C XC ACCUMMULATION OF INTERMEDIATE
C

```

1  FORMAT(5F15.0)
2  FORMAT(7F10.0)
3  FORMAT(17X,7F10.4)
4  FORMAT(7I4)
5  FORMAT(3F10.0)
6  FORMAT(20X,7F10.3)
7  FORMAT(31X,3F15.5)
8  FORMAT(19X,3F10.5,2F9.3,F12.4,F8.3)
9  FORMAT(18X,5F15.5)
10 FORMAT(18X,10I10)
432 FORMAT(10X,28HENERGY BALANCE DID NOT MATCH)
433 FORMAT(/45X,24HINITIAL CONDITION VECTOR/)
434 FORMAT(/45X,25HBOUNDARY CONDITION VECTOR/)
435 FORMAT(/50X,8HMATRIX G/)
436 FORMAT(/50X,8HMATRIX B/)
437 FORMAT(/47X,18HKINETIC PARAMETERS/)
438 FORMAT(/20X,41HINITIAL CONDITION FOR GAS PHASE
    * EQUATIONS/)
491 FORMAT(1H1)
492 FORMAT(/20X,20HPARTICLE DIAMETER = ,F6.2,3X
    *,16HLOADING RATIO = ,F
    24.1,3X,17HSCALING FACTOR = ,F6.1)
493 FORMAT(/22X,2HXA,9X,2HXB,9X,2HXC,9X,2HVG,7X,2HVP,6X
    *,2HTG,7X,2HDL)
494 FORMAT(/20X,4HT(1),7X,4HT(2),6X,4HT(3),6X,4HT(4),6X
    *,4HT(5),6X,2HTS
    2,9X,3HDIF/)
495 FORMAT(1X,////)
499 FORMAT(28X,20HPARTICLE DIAMETER = ,F6.2,3X,16HLOADING
    * RATIO = ,F4.
    21)
531 FORMAT(20X,7F10.4)
710 FORMAT(7F10.0)
711 FORMAT(/20X,19HGAS PHASE CONSTANTS//18X,5F15.5)
712 FORMAT(/20X,29HPROPERTIES OF SOLID PARTICLES//18X
    *,5F15.5)
714 FORMAT(/20X,44HPOLYNOMIAL COEFFICIENTS FOR WALL
    * TEMPERATURE//18X,
    25F15.5)
805 FORMAT(10X,4E18.5)
    WRITE(6,495)

```

```

READ(5,4)N3,N4,M,N,MM,MP,ML
WRITE(6,10)N3,N4,M,N,MM,MP,ML
READ(5,4)MG,MT,MR,NGT,NPT,KQT

```


C TBR ... (CONT'D)

WRITE(6,10)MG,MT,MR,NGT,NPT,KQT

C READ IN CONSTANTS

C

READ(5,2)PR,RR,GC,FR,FL,DRR,ZO
WRITE(6,6)PR,RR,GC,FR,FL,DRR,ZO
READ(5,2)TB,HR,FIF,ES,C,TO
WRITE(6,6)TB,HR,FIF,ES,C,TO

C READ IN REACTION PARAMETERS

C

READ(5,5)(EA(I),AA(I),W(I),I=1,M)
WRITE(6,437)
WRITE(6,7)(EA(I),AA(I),W(I),I=1,M)

C READ IN INITIAL CONDITION FOR GAS PHASE EQUATIONS

C

READ(5,2)(TI(I),I=1,MM)

C READ IN MATRICES AND VECTORS FOR SOLIDS PDE

C

READ(5,1)((G(I,J),J=1,N),I=1,N)
WRITE(6,435)
WRITE(6,9)((G(I,J),J=1,N),I=1,N)
READ(5,1)((B(I,J),J=1,N),I=1,N)
WRITE(6,436)
WRITE(6,9)((B(I,J),J=1,N),I=1,N)
READ(5,1)(UO(I),I=1,N)
WRITE(6,433)
WRITE(6,9)(UO(I),I=1,N)
READ(5,1)(U(I),I=1,N)
WRITE(6,434)
WRITE(6,9)(U(I),I=1,4)
WRITE(6,491)
WRITE(6,495)

C DO THE MATRIX CALCULATIONS
C FIND EIGENVALUES AND EIGENVECTORS

C

CALL CLMT(G,B,V,A,N)
GD=GC*RR
HR=HR*1000.0
FN3=N3
FN4=N4
DRR=DRR/12.0

1. Introduction

The following table shows the results of the experiment.

Table 1: Results of the experiment

Results of the experiment for different values of the parameter α .

Results of the experiment for different values of the parameter β .

Results of the experiment for different values of the parameter γ .

Results of the experiment for different values of the parameter δ .

Results of the experiment for different values of the parameter ϵ .

Results of the experiment for different values of the parameter ζ .

Results of the experiment for different values of the parameter η .

Results of the experiment for different values of the parameter θ .

Results of the experiment for different values of the parameter ι .

C TBR

... (CONT'D)

ARR=0.785*DRR**2
AW=3.1417*DRR
DZ=FL/FN4

C START THE CALCULATIONS
C

DO 600 LG=1, MG

C READ IN THE CONSTANTS FOR GAS PHASE
C

READ (5,710)WQ,WM,TGO,TO
WRITE(6,711)WQ,WM,TGO,TO
RR=RR/WM

C READ IN PROPERTIES OF MATERIALS OF THE SOLID
C PARTICLES
C

DO 600 LT=1, MT
READ(5,710)DS,CS,SK
WRITE(6,712)DS,CS,SK
AL=SK/(DS*CS)

C READ IN THE PARTICLE DIAMETER, INITIAL PARTICLE
C PARTICLE
C VELOCITY AND THE PERTURBATION FACTOR
C

DO 600 LR=1, MR
READ(5,710) RA,VPO,FT
DP=2.0*RA

C READ IN THE LOADING RATIO
C

DO 600 LK=1, ML
READ(5,710)SOG
WP=SOG*WQ

C READ IN THE POLYNOMIAL COEFFICIENTS FOR WALL
C TEMPERATURE
C

READ (5,710)A1,A2,A3,A4
WRITE(6,714)A1,A2,A3,A4

WRITE(6,492)DP,SOG,FT

... 10000

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C

TBR

...(CONT'D)

```

FTO=FT
GM=WQ/WM
WG=WQ/ARR
GS=WG/WM
B3=0.05*GM*HR
RA=RA*3.28E-06
DR=RA/FN3
DO 13 I=1,N
FI=I-1
13 R(I)=FI*DR
DO 14 I=1,N
TN(I)=TO-460.0
TT(I)=TO
14 CONTINUE
DST=TO
XO=0.0
IA=1
DO 18 I=1,N
18 T(IA,I)=TO
DG=(WM*PR)/(10.73*TGO)
VG=WG/DG
VG=VG/3600.0
TI(7)=VG
WRITE(6,438)
WRITE(6,531)(TI(I),I=1,MM)
WRITE(6,491)
WRITE(6,495)
WRITE(6,499) DP,SOG
DP=DP*3.28E-06
TI(4)=TGO/TB
TI(6)=VPO
TI(5)=TO/TB
DO 31 I=1,MM
TY(I)=TI(I)
31 CONTINUE
WS=WP/ARR
CK=3.0*WP*CS*DZ
CAD=0.20*DG/WM
CBO=0.05*DG/WM
VP=TY(6)
TG=TY(4)*TB
TP=TY(5)*TB
DSTP=DST-460.0
TGP=TGO-460.0
DF=TGP-DSTP
LP=0
WRITE(6,493)
WRITE(6,494)
WRITE(6,8)TI(1),TI(2),TI(3),TI(7),TI(6),TGP,XO
WRITE(6,3)(TN(I),I=1,N),DSTP,DF

```


C TBR

C TBR

```

503 DG=(WM*PR)/(10.73*TG)
    CPG=0.1903+1.8E-04*TG-3.147E-08*TG**2
    UG=0.04598+0.00004556*(TG-660.0)
    TKG=0.01762+0.0000233*(TG-660.0)
    HW=0.16*TKG/DRR*(WS/WG)**0.45*(DRR*WG/UG)**0.6*(CPG*UG
*/TKG)**0.4
    HC=0.16*(TKG/DP)*(DP*WG/UG)**0.5
    UG=UG/3600.0
    VT=(2.4*(DS-DG)**0.673*DP**1.02)/(DG**0.327*UG**0.347)
    STG=SOG*VG/VP
    E=STG*DG/DS
    E=1.0-E

```

C CONSTANTS FOR ENERGY EQUATIONS

C

```

F1=(4.0*HW)/(DRR*CPG*WG)
F3=(0.05*HR)/(CPG*WM)
F6=E/(0.05*GS)
F3=F3/TB
B1=HW*AW
B4=12.0*DR*HC/SK
B2=DG/WG

```

C CONSTANTS FOR MOMENTUM EQUATIONS

C

```

UGU=ABS(VG-VP)
RNP=DP*DG*UGU/UG
RNP=SQRT(RNP)
CD=0.64+4.8/RNP
CD=CD**2
FF1=0.75*CD*DG*UGU/(DP*DS)
C8=VP*RA*RA*3600.0*RA
CP=CK/C8
DT=DZ/(VP*3600.0)
DTM=AL*DT/DR
DTM=DTM/DR
DC=DTM
AS=6.0*WP/(VP*DP*DS*3600.0)
F2=STG*CS/CPG
F4=VP*DS*CS*DP*3600.0
F5=6.0*HC/F4
F7=HC*AS*DZ*DT
103 P=T(IA,N)
    TS=B4*TG+18.0*T(IA,N-1)-9.0*T(IA,N-2)+2.0*T(IA,N-3)
    TS=TS/(11.0+B4)
    C5=TG*CPG*WM
    KQ=0

```


C TBR ... (CONT'D)

$F = (TS - P) / DTM$

IN=0

IP=0

100 KQ=KQ+1

IF(IN-NGT)105,105,65

105 IF(IP-NPT)102,102,65

C SOLVE THE GAS PHASE DIFFERENTIAL EQUATIONS

C

102 CALL GENER(TY,D,W,AA,EA,XO,DZ,MM,M,P,F,DC,STG,TW)

C OBTAIN THE ENTHALPY BALANCE FOR THE GAS PHASE

C

$C4 = D(4) * TB * CPG * WM$

$Q2 = ((C5 - C4) * GM - B1 * DZ * (D(4) - TW) * TB + B3 * (D(2) - TY(2))) * DT$

C CALL THE SUBROUTINES FOR CALCULATION OF SOLIDS

C

TEMPERATURES

C

AND SOLIDS ENTHALPY BALANCE

C

CALL SIMPS(N,F,P,DTM,A,TC2,G)

CALL TMDEF(B,V,G,T,TT,Q1,R,TS,DR,CP,DTM,IA,N,A,TC2)

IF(Q1)407,408,408

C MATCH THE SOLIDS AND GAS ENTHALPT BALANCES

C

408 TES= ABS(Q1-Q2)

AQ= ABS(Q1+Q2)

TES=TES*2.0/AQ

IF(TES-ES)50,50,412

412 Q3=(Q1+Q2)/2.0

$Q5 = F7 * (D(4) * TB - P - F * 0.5 * DTM)$

$QC = Q3 / F7$

$F = (D(4) * TB - P - QC) / (0.5 * DTM)$

IF(KQ-KQT)410,410,407

C PERTURB THE MATCHING FACTOR

C

410 F=F/FT

GO TO 100

C SEARCH FOR THE MATCHING FACTOR

C

407 FT=FT+0.01*FT

C

TBR

... (CONT'D)

F=F/FT
 IN=IN+1
 KQ=0
 GO TO 100

C MATCHING HAS BEEN OBTAINED
 C

50 TY(1)=D(1)
 TY(2)=D(2)
 TY(3)=D(3)
 TY(4)=D(4)
 TY(5)=D(5)
 TY(6)=D(6)
 TY(7)=D(7)
 XO=XO+DZ
 TG=TY(4)*TB
 TP=TY(5)*TB
 DST=F*DTM+P
 IA=IA+1
 DO 46 I=1,N
 46 T(IA,I)=TT(I)
 DO 77 I=1,N
 TN(I)=TT(I)-460.0
 77 CONTINUE
 TGP=TG-460.0
 DSTP=DST-460.0
 DF=TG-DST
 VP=TY(6)
 VG=TY(7)
 TWB=TW*TB-460.0
 IF(DF.LT.20.0) GO TO 579
 LN=-1
 GO TO 581
 579 LN=0
 581 IF(IA.GT.N4) GO TO 66
 LP=LP+1
 IF(LP.EQ.10) GO TO 507
 GO TO 509
 507 WRITE(6,8)TY(1),TY(2),TY(3),VG,VP,TGP,XO
 WRITE(6,3)(TN(I),I=1,N),DSTP,DF
 LP=0
 509 IF(LN.EQ.0) GO TO 517
 ES=0.05
 GO TO 503
 517 ES=0.10
 GO TO 503
 65 WRITE(6,8)TY(1),TY(2),TY(3),VG,VP,TGP,XO
 WRITE(6,3)(TN(I),I=1,N),DSTP,DF
 WRITE(6,491)

C TBR ... (CONT'D)

```
WRITE(6,432)
66 GO TO 600
600 CONTINUE
CALL EXIT
END
```


SUBROUTINE CLMT

SUBROUTINE CLMT(G,B,V,A,N)

C THIS SUBROUTINE CALCULATES THE CONSTANTS IN THE
 C SOLUTION
 C OF THE MATRIX DIFFERENTIAL EQUATION.
 C

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
 COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CAO,CBO
 DIMENSION G(12,12),B(12,12),V(12,12),GG(12,12),G1(12
 *,12)
 DIMENSION QT(12,12),QP(12,12),A(78),Q(78),AR(12)

9 FORMAT(18X,5F15.6)
 41 FORMAT(//50X,8HMATRIX K/)
 42 FORMAT(//50X,11HEIGENVALUES/)
 43 FORMAT(//50X,12HEIGENVECTORS/)

DO 10 I=1,N
 DO 10 J=1,N
 IF(I-J)11,12,11
 11 GG(I,J)=0.0
 G1(I,J)=0.0
 G(I,J)=0.0
 GO TO 10
 12 G(I,I)=G(I,I)
 GG(I,I)=1.0/(SQRT(G(I,I)))
 G1(I,I)=SQRT(G(I,I))
 10 CONTINUE

C CALCULATE MATRIX K
 C

CALL GMPRD(GG,B,V,N,N,N)
 CALL GMPRD(V,GG,B,N,N,N)
 WRITE(6,41)
 WRITE(6,9)((B(I,J),J=1,N),I=1,N)

C CONVERT MATRIX K TO STORAGE MODE 1
 C

JJ=1
 DO 21 J=1,N
 DO 21 I=1,J
 A(JJ)=B(I,J)
 JJ=JJ+1
 21 CONTINUE

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SUBROUTINE CLMT ... (CONT'D)

C FIND EIGENVALUES OF MATRIX K
C

MV=0
CALL EIGEN(A,Q,N,MV)

C SORT OUT EIGENVALUES
C

JJ=1
DO 22 I=1,N
IF(I-1)15,15,16
16 JJ=JJ+I
15 A(I)=A(JJ)
AR(I)=1.0/A(I)
22 CONTINUE
WRITE(6,42)
WRITE(6,9)(A(I),I=1,N)

C SORT OUT EIGENVECTORS
C

DO 19 J=1,N
DO 19 I=1,N
JK=(J-1)*N+I
QP(I,J)=Q(JK)
QT(J,I)=QP(I,J)
19 CONTINUE
WRITE(6,43)
WRITE(6,9)((QP(I,J),J=1,N),I=1,N)
CALL GMPRD(GG,QP,B,N,N,N)
CALL GMPRD(QT,G1,V,N,N,N)
CALL GMPRD(QT,GG,G,N,N,N)
RETURN
END

SUBROUTINE EIGEN

SUBROUTINE EIGEN(A,R,N,MV)

C THIS SUBROUTINE CALCULATES THE EIGENVALUES AND
 C EIGENVECTORS
 C OF A SYMMETRIC MATRIX BY THE METHOD OF JACOBI. THIS
 C ROUTINE
 C IS REPRODUCED FROM IBM SCIENTIFIC SUBROUTINE
 C PACKAGE.

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
 COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CA0,CB0
 DIMENSION A(78),R(78)

C GENERATE IDENTITY MATRIX

C 5 RANGE=1.0D-12

5 RANGE=1.0E-12
 IF(MV-1) 10,25,10
 10 IQ=-N
 DO 20 J=1,N
 IQ=IQ+N
 DO 20 I=1,N
 IJ=IQ+I
 R(IJ)=0.0
 IF(I-J) 20,15,20
 15 R(IJ)=1.0
 20 CONTINUE

C COMPUTE INITIAL AND FINAL NORMS (ANORM AND ANORMX)
 C

25 ANORM=0.0
 DO 35 I=1,N
 DO 35 J=I,N
 IF(I-J) 30,35,30
 30 IA=I+(J-J)/2
 ANORM=ANORM+A(IA)*A(IA)
 35 CONTINUE
 IF(ANORM) 165,165,40

C 40 ANORM=1.414*DSQRT(ANORM)

40 ANORM=1.414* SQRT(ANORM)
 ANRMX=ANORM*RANGE/FLOAT(N)

C INITIALIZE INDICATORS AND COMPUTE THRESHOLD, THR
 C

100000 - 100000

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SUBROUTINE EIGEN ... (CONT'D)

```

      IND=0
      THR=ANORM
45  THR=THR/FLOAT(N)
50  L=1
55  M=L+1

C      COMPUTE SIN AND COS
C
60  MQ=(M*M-M)/2
      LQ=(L*L-L)/2
      LM=L+MQ
C 62  IF(DABS(A(LM))-THR) 130,65,65
62  IF( ABS(A(LM))-THR) 130,65,65
65  IND=1
      LL=L+LQ
      MM=M+MQ
      X=0.5*(A(LL)-A(MM))
68  Y=-A(LM)/ SQRT(A(LM)*A(LM)+X*X)
      IF(X) 70,75,75
70  Y=-Y
C 75  SINX=Y/DSQRT(2.0*(1.0+(DSQRT(1.0-Y*Y))))
75  SINX=Y/ SQRT(2.0*(1.0+( SQRT(1.0-Y*Y))))
      SINX2=SINX*SINX
C 78  COSX=DSQRT(1.0-SINX2)
78  COSX= SQRT(1.0-SINX2)
      COSX2=COSX*COSX
      SINCS =SINX*COSX
C      ROTATE L AND M COLUMNS
C
      ILQ=N*(L-1)
      IMQ=N*(M-1)
      DO 125 I=1,N
      IQ=(I*I-I)/2
      IF(I-L) 80,115,80
80  IF(I-M) 85,115,90
85  IM=I+MQ
      GO TO 95
90  IM=M+IQ
95  IF(I-L) 100,105,105
100 IL=I+LQ
      GO TO 110

```

$$\frac{1}{2} \sqrt{1 - \frac{1}{2}} = 0.41 \quad (2)$$
[illegible]

20, 20, 051 (941-1 (011) 20A) 20 9A

1-100 200

$$G_1 + G_2 = G$$
$$f(1999) - f(1998) = 2000, f(1998) - f(1997) = 2000, \dots, f(1999) - f(1998) = 2000$$
$$(1, 2) + (-1, 1) = (0, 3) \text{ and } (1, 2) + (-2, 1) = (-1, 3) \text{ and}$$

1981.05.05

$$Y = Y - 0.5$$
$$((Y \leq Y_{(1-n)}), 1)T = 2(1) = 1, (1) = 0, (0) = 2(0 \setminus Y = x_{(1)} = 2) = 1$$
$$1.01 \text{ FACTOR} 2 = \text{CYM} 1.2$$
$$(\sin x)^2 = 1 - (\cos x)^2 = 1 - \frac{1}{2} = \frac{1}{2} \quad \text{or} \quad \sin x = \pm \frac{1}{\sqrt{2}}.$$
$$(1.4972 - 11.1) (102) = 820.745$$

1993年12月20日=98/20日

21902 = 25912

$$(1 - \frac{1}{2}) \times 100 = 50\%$$

() - M } 2000/1/1

$$M_n \equiv \int_0^{\infty} \tau^n f(\tau) d\tau$$
$$S \setminus (I - I_0) = \emptyset$$

08.11.04 (1-12)

$$0, 3, 1, 2, n \quad (n-1) \geq 1$$

1994-1-11

1990-1991

$$I + \dots = 1$$

201, 202, 203 (1-1) 91

$$0 + 1 = 1$$

011 07 03

SUBROUTINE EIGEN ... (CONT'D)

```

105 IL=L+IQ
110 X=A(IL)*COSX-A(IM)*SINX
    A(IM)=A(IL)*SINX+A(IM)*COSX
    A(IL)=X
115 IF(MV-1) 120,125,120
120 ILR=ILQ+I
    IMR=IMQ+I
    X=R(ILR)*COSX-R(IMR)*SINX
    R(IMR)=R(ILR)*SINX+R(IMR)*COSX
    R(ILR)=X
125 CONTINUE
    X=2.0*A(LM)*SINCS
    Y=A(LL)*COSX2+A(MM)*SINX2-X
    X=A(LL)*SINX2+A(MM)*COSX2+X
    A(LM)=(A(LL)-A(MM))*SINCS+A(LM)*(COSX2-SINX2)
    A(LL)=Y
    A(MM)=X

```

```

C      TESTS FOR COMPLETION
C
C      TEST FOR M = LAST COLUMN
C

```

```

130 IF(M-N) 135,140,135
135 M=M+1
    GO TO 60

```

```

C      TEST FOR L = SECOND FROM LAST COLUMN
C

```

```

140 IF(L-(N-1)) 145,150,145
145 L=L+1
    GO TO 55
150 IF(IND-1) 160,155,160
155 IND=0
    GO TO 50

```

```

C      COMPARE THRESHOLD WITH FINAL NORM
C

```

```

160 IF(THR-ANRMX) 165,165,45

```

```

C      SORT EIGENVALUES AND EIGENVECTORS
C

```

```

165 IQ=-N
    DO 185 I=1,N
        IQ=IQ+N
        LL=I+(I*I-I)/2
        JQ=N*(I-2)

```


SUBROUTINE EIGEN ... (CONT'D)

```
DO 185 J=I,N
  JQ=JQ+N
  MM=J+(J*J-J)/2
  IF(A(LL)-A(MM)) 170,185,185
170 X=A(LL)
  A(LL)=A(MM)
  A(MM)=X
  IF(MV-1) 175,185,175
175 DO 180 K=1,N
  ILR=IQ+K
  IMR=JQ+K
  X=R(ILR)
  R(ILR)=R(IMR)
180 R(IMR)=X
185 CONTINUE
  RETURN
END
```


SUBROUTINE TMDEF

SUBROUTINE TMDEF(B,V,G,T,TT,Q1,R,TS,DR,CP,DTM,IA,N,A
*,TC2)

```

C      THIS SUBROUTINE CALCULATES THE INITIAL VALUE
C      CONTRIBUTION
C      TO THE TEMPERATURE DISTRIBUTION IN THE SOLID
C      PARTICLES.
C      IT ALSO INTEGRATES THE TEMPERATURE DISTRIBUTION
C      THROUGHOUT
C      THE ENTIRE VOLUME OF THE PARTICLES IN ORDER TO
C      OBTAIN THE
C      HEAT RECEIVED BY THE PARTICLES.
C
C      DOUBLE PRECISION Y

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CAO,CBO
DIMENSION TT(12),R(12),Y(12)
DIMENSION B(12,12),G(12,12),V(12,12),T(200,12)
DIMENSION UO(12),      TC1(12),TC2(12),      A(78)
*,TC(12)

FIF=160.0
IP=IA
DO 10 I=1,N
  UO(I)=T(IA,I)
10 CONTINUE
  CALL GMVRD(V,UO,TC1,N,N,1)
  DO 19 I=1,N
    ECT=A(I)*DTM
    IF(ECT-FIF)39,39,33
39  ECT= EXP(ECT)
    GO TO 34
33  ECT=0.0
34  TC1(I)=TC1(I)*ECT
    TC(I)=TC1(I)+TC2(I)
19 CONTINUE
  CALL GMVRD(B,TC,TT,N,N,1)
  IP=IP+1
  DO 73 I=1,N
    T(IP,I)=TT(I)
73 CONTINUE
  DO 57 K=1,N
    Y(K)=(T(IP,K)-T(IA,K))*R(K)*R(K)
57 CONTINUE
  A21=DR*2.0*(Y(1)+4.0*Y(3)+Y(5))/3.0
  A22=DR*(Y(1)+4.0*Y(2)+2.0*Y(3)+4.0*Y(4)+Y(5))/3.0
  A23=(A22-A21)/15.0
  SB=A22+A23

```


SUBROUTINE TMDEF ... (CONT'D)

Q1=CP*SB

TS=TT(N)

RETURN

END

SUBROUTINE SIMPS

SUBROUTINE SIMPS(N,F,P,DTM,A,TC2,G)

C THIS SUBROUTINE CALCULATES THE BOUNDARY VALUE
 C CONTRIBUTION
 C TO THE TEMPERATURE DISTRIBUTION IN THE SOLID
 C PARTICLES
 C

```

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CAO,CBO
DIMENSION G(12,12),A(78),TC2(12)
FIF=160.0
DO 211 I=1,N
  ECT=A(I)*DTM
  IF(ECT-FIF)39,39,33
39  ECT= EXP(ECT)
  GO TO 38
33  ECT=0.0
38  EPT=ECT-1.0
  BC=((P+F/A(I))*EPT-F*DTM)*G(I,5)/A(I)*81.0
  TC2(I)=BC
211 CONTINUE
  RETURN
  END

```


SUBROUTINE GMPRD

SUBROUTINE GMPRD(X,Y,Z,L,M,ML)

C
C

THIS SUBROUTINE MULTIPLIES TWO MATRICES.

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
 COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CAO,CBO
 DIMENSION X(12,12),Y(12,12),Z(12,12)

DO 21 I=1,L
 DO 21 J=1,L
 SUM=0.0
 DO 22 K=1,L
 SUM=SUM+X(I,K)*Y(K,J)
 22 CONTINUE
 Z(I,J)=SUM
 21 CONTINUE
 RETURN
 END

SUBROUTINE GMVRD

SUBROUTINE GMVRD(X,Y,Z,L,M,ML)

C THIS SUBROUTINE MULTIPLIES A VECTOR WITH A MATRIX.
C

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CAO,CBO
DIMENSION X(12,12),Y(12),Z(12)

DO 23 I=1,L
SUM=0.0
DO 24 K=1,L
SUM=SUM+X(I,K)*Y(K)
24 CONTINUE
Z(I)=SUM
23 CONTINUE
RETURN
END

SUBROUTINE GENER

SUBROUTINE GENER(TY,D,W,AA,EA,XO,DZ,MM,M,P,F,DC,STG
*,TW)

C THIS SUBROUTINE SOLVES THE GAS PHASE EQUATIONS BY
C RUNGE-KUTTA METHOD.
C

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CAO,CBO
REAL KP
DIMENSION TY(8),D(8),W(8),AA(8),EA(8)
DIMENSION DE(8),KP(4,8)

DO 101 II=1,4
GOTO(102,103,104,105),II
102 XL=XO
DO 106 I=1,MM
106 D(I)=TY(I)
GO TO 107
103 XL=XO+0.5*DZ
DO 108 I=1,MM
108 D(I)=TY(I)+0.5*KP(1,I)
GO TO 107
104 DO 109 I=1,MM
109 D(I)=TY(I)+KP(2,I)
GO TO 107
105 XL=XO+DZ
DO 110 I=1,MM
110 D(I)=TY(I)+KP(3,I)
107 CALL SLOPE(D,W,AA,EA,XL,DE,P,F,DC,STG,TW,M)
DO 101 I=1,MM
101 KP(II,I)=DZ*DE(I)
DO 100 I=1,MM
100 D(I)=TY(I)+(KP(1,I)+KP(4,I)+2.0*(KP(2,I)+KP(3,I)))/6.0
RETURN
END

SUBROUTINE SLOPE

SUBROUTINE SLOPE(D,W,AA,EA,XL,DE,P,F,DC,STG,TW,M)

C
C

THIS SUBROUTINE CALCULATES THE FUNCTIONS.

COMMON A1,A2,A3,A4,C,TB,GC,GD,DRR,FR
COMMON F1,F2,F3,F5,FF1,B2,B5,B6,CAO,CBO
DIMENSION D(8),W(8),AA(8),EA(8),DE(8),QR(8)

XQ=XL/10.0
TW=A1+A2*XQ+A3*XQ**2+A4*XQ**3
TG=D(4)*TB
DO 10 I=1,M
10 QR(I)=W(I)*EXP(AA(I)-EA(I)*C/TG)
C1=QR(1)*(1.0-D(1))*(1.0-D(2))
C3=QR(2)*(1.0-D(2))*D(3)
C7=QR(3)*(1.0-D(1))
DE(1)=B2*(C1*CBO*(1.0+2.0*CAO*C7)+C3*C7*CAO*CBO)
DE(2)=B2*(2.0*C1*CAO+C3*CAO)*(1.0+C7*CAO)
DE(3)=B2*(C1*CBO*(1.0+2.0*CAO*C7)+C3*CBO*(C7*CAO-1.0))
DE(4)=-F1*(D(4)-TW)-F2*F5*(D(4)-P/TB-F/TB*0.5*DC)+F3
**DE(2)
DE(5)=F5*(D(4)-D(5))
DE(6)=FF1*(D(7)-D(6))/D(6)
DE(6)=DE(6)+GC/D(6)
B6=STG*D(6)/(GD*D(4)*TB)
B5=GD*D(4)*DRR*TB
CM=DE(4)/D(4)+B6*DE(6)+2.0*D(7)**2*FR/B5
CM=CM+(1.0+STG)/(GD*D(4)*TB)
DN=1.0/D(7)-D(7)/(GD*D(4)*TB)
DE(7)=CM/DN
RETURN
END

5	180	3	5	7	5	1
1	1	1	5	5	60	
50.000	1545.000	32.200	0.001	9.000	0.625	0.0
1190.000	150.000	150.000	0.050	506.000	1140.000	

KINETIC PARAMETERS

48.00000	34.50000	0.00010
25.00000	35.20000	0.00010
-25.00000	9.90000	0.00010

MATRIX G

0.16665	0.0	0.0	0.0	0.0
0.0	4.33330	0.0	0.0	0.0
0.0	0.0	16.33330	0.0	0.0
0.0	0.0	0.0	36.33330	0.0
0.0	0.0	0.0	0.0	64.33330

MATRIX B

-1.00000	1.00000	0.0	0.0	0.0
1.00000	-10.00000	9.00000	0.0	0.0
0.0	9.00000	-34.00000	25.00000	0.0
0.0	0.0	25.00000	-74.00000	49.00000
0.0	0.0	0.0	49.00000	-130.00000

INITIAL CONDITION VECTOR

1140.00000	1140.00000	1140.00000	1140.00000	1140.00000
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BOUNDARY CONDITION VECTOR

0.0	0.0	0.0	0.0
-----	-----	-----	-----

MATRIX K

-6.000241	1.176725	0.0	0.0	0.0
1.176725	-2.307711	1.069784	0.0	0.0
0.0	1.069784	-2.081636	1.026243	0.0
0.0	0.0	1.026243	-2.036697	1.013504
0.0	0.0	0.0	1.013504	-2.020724

EIGENVALUES

-0.379675	-1.379019	-2.637214	-3.684029	-6.367013
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EIGENVECTORS

0.079721	-0.151063	0.194053	-0.166582	0.951534
0.380786	-0.593252	0.554592	-0.327891	-0.206591
0.598587	-0.348836	-0.384230	0.605085	0.078768
0.595777	0.379596	-0.370077	-0.602949	-0.019745
0.367949	0.599541	0.608392	0.367423	0.004604

GAS PHASE CONSTANTS

12.00000	50.00000	1190.00000	1140.00000
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PROPERTIES OF SOLID PARTICLES

197.00000	0.20000	9.00000
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POLYNOMIAL COEFFICIENTS FOR WALL TEMPERATURE

0.99939	-0.27840	1.59250	-1.30014
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PARTICLE DIAMETER = 100.00 LOADING RATIO = 5.0 SCALING FACTOR = 0.0

INITIAL CONDITION FOR GAS PHASE EQUATIONS

0.0	0.0	0.0	1.0000	0.9500	8.8000	7.9950
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PARTICLE DIAMETER = 100.00 LOADING RATIO = 5.0

XA	XB	XC	VG	VP	TG	DL
T(1)	T(2)	T(3)	T(4)	T(5)	TS	DIF
0.0	0.0	0.0	7.995	8.800	730.0000	0.0
680.0000	680.0000	680.0000	680.0000	680.0000	680.0000	50.0000
0.00009	0.00038	0.00009	7.843	9.069	707.3618	0.500
700.1086	700.1152	700.1238	700.1299	700.1328	700.1328	7.2290
0.00036	0.00145	0.00036	7.838	9.094	706.6128	1.000
704.0925	704.0991	704.1069	704.1118	704.1125	704.1108	2.5026
0.00112	0.00452	0.00110	7.852	9.105	708.6499	1.500
706.3340	706.3408	706.3486	706.3535	706.3542	706.3521	2.2979
0.00325	0.01316	0.00321	7.884	9.127	713.5244	2.000
709.4758	709.4824	709.4910	709.4961	709.4978	709.4961	4.0233
0.00904	0.03663	0.00891	7.950	9.171	723.3735	2.500
715.4236	715.4302	715.4387	715.4448	715.4482	715.4485	7.9250
0.02344	0.09520	0.02309	8.075	9.257	741.8787	3.000
726.8057	726.8132	726.8237	726.8313	726.8372	726.8411	15.0376
0.05334	0.21725	0.05237	8.279	9.403	772.3000	3.500
746.7075	746.7156	746.7268	746.7373	746.7466	746.7546	25.5454
0.09913	0.40565	0.09685	8.530	9.618	809.6658	4.000
775.8257	775.8342	775.8472	775.8601	775.8728	775.8853	33.7805
0.14795	0.60863	0.14375	8.742	9.836	841.2300	4.500
808.4939	808.5029	808.5166	808.5300	808.5422	808.5544	32.5755
0.18621	0.76932	0.18010	8.872	10.000	860.5500	5.000
835.9434	835.9512	835.9639	835.9753	835.9846	835.9929	24.5571
0.21074	0.87307	0.20321	8.943	10.101	871.0906	5.500
855.2561	855.2642	855.2751	855.2839	855.2905	855.2954	15.7952
0.22478	0.93275	0.21635	8.983	10.162	877.8010	6.000
867.8108	867.8186	867.8286	867.8359	867.8403	867.8418	9.9592
0.23236	0.96506	0.22345	9.022	10.203	882.8320	6.500
875.9878	875.9949	876.0044	876.0115	876.0139	876.0142	6.8176
0.23632	0.98203	0.22715	9.048	10.233	886.6951	7.000
881.7234	881.7305	881.7405	881.7466	881.7435	881.7473	4.9474
0.23837	0.99080	0.22905	9.063	10.254	888.5512	7.500
885.6643	885.6721	885.6812	885.6875	885.6887	885.6863	3.2133
0.23942	0.99530	0.23003	9.062	10.262	888.6868	8.000
887.6091	887.6165	887.6250	887.6306	887.6311	887.6274	1.0593
0.23956	0.99589	0.23016	9.058	10.262	888.2363	8.100
887.6882	887.6956	887.7034	887.7083	887.7080	887.7043	0.5320

PARTICLE DIAMETER = 200.00 LOADING RATIO = 5.0

XA	XP	XC	VG	VP	TG	DL
T (1)	T (2)	T (3)	T (4)	T (5)	TS	DIF
0.0	0.0	0.0	7.995	8.800	730.0000	0.0
680.0000	680.0000	680.0000	680.0000	680.0000	680.0000	50.0000
0.00010	0.00040	0.00010	7.894	9.887	714.9316	0.500
690.8000	690.8076	690.8193	690.8313	690.8425	690.8538	24.0779
0.00037	0.00151	0.00037	7.855	10.426	709.2112	1.000
695.7332	695.7400	695.7500	695.7581	695.7642	695.7693	13.4419
0.00116	0.00469	0.00115	7.853	10.698	708.8123	1.500
698.7141	698.7212	698.7310	698.7383	698.7424	698.7456	10.0667
0.00337	0.01364	0.00333	7.888	10.848	714.0493	2.000
701.5530	701.5598	701.5696	701.5776	701.5828	701.5872	12.4622
0.00934	0.03786	0.00921	7.974	10.954	726.8984	2.500
705.6917	705.6992	705.7112	705.7214	705.7312	705.7395	21.1589
0.02405	0.09771	0.02367	8.137	11.068	751.1665	3.000
712.6042	712.6133	712.6279	712.6433	712.6594	712.6765	38.4900
0.05401	0.22035	0.05294	8.397	11.224	789.8145	3.500
724.7339	724.7434	724.7632	724.7869	724.8147	724.8467	64.9678
0.09898	0.40636	0.09637	8.704	11.435	835.5613	4.000
743.6829	743.6953	743.7205	743.7537	743.7937	743.8425	91.7188
0.14643	0.60541	0.14151	8.945	11.668	871.4141	4.500
767.8730	767.8867	767.9150	767.9534	768.0020	768.0601	103.3540
0.18380	0.76414	0.17657	9.069	11.870	889.9011	5.000
792.4910	792.5042	792.5317	792.5681	792.6128	792.6670	97.2341
0.20812	0.86823	0.19920	9.116	12.014	896.7876	5.500
814.1538	814.1663	814.1909	814.2231	814.2615	814.3074	82.4802
0.22231	0.92916	0.21234	9.136	12.107	899.8403	6.000
831.9885	832.0002	832.0215	832.0488	832.0801	832.1172	67.7231
0.23010	0.96269	0.21954	9.156	12.168	902.7979	6.500
846.4778	846.4888	846.5085	846.5325	846.5591	846.5889	56.2090
0.23424	0.98056	0.22336	9.177	12.211	905.9199	7.000
858.4922	858.5024	858.5198	858.5400	858.5625	858.5869	47.3330
0.23641	0.98992	0.22535	9.190	12.242	907.7981	7.500
868.3997	868.4092	868.4250	868.4426	868.4600	868.4795	39.3186
0.23754	0.99479	0.22638	9.181	12.261	906.5339	8.000
876.2117	876.2212	876.2356	876.2498	876.2632	876.2764	30.2576
0.23812	0.99731	0.22692	9.139	12.260	900.2534	8.500
881.4949	881.5034	881.5156	881.5256	881.5334	881.5393	18.7141

55.858 FC=0

PARTICLE DIAMETER = 300.00 LOADING RATIO = 5.0

XA	XB	XC	VG	VP	TG	DL
T(1)	T(2)	T(3)	T(4)	T(5)	TS	DIF
0.0	0.0	0.0	7.995	8.300	730.0000	0.0
680.0000	680.0000	680.0000	680.0000	680.0000	680.0000	50.0000
0.00010	0.00041	0.00010	7.917	10.149	718.3623	0.500
686.6074	686.6167	686.6311	686.6482	686.6667	686.6870	31.6755
0.00038	0.00154	0.00038	7.868	11.018	711.1460	1.000
690.2295	690.2373	690.2493	690.2615	690.2729	690.2847	20.8613
0.00117	0.00476	0.00116	7.857	11.585	709.4321	1.500
692.6042	692.6121	692.6230	692.6340	692.6433	692.6526	16.7795
0.00341	0.01381	0.00337	7.894	11.969	714.9829	2.000
694.8340	694.8423	694.8547	694.8665	694.8772	694.8879	20.0950
0.00943	0.03826	0.00930	7.997	12.249	730.3301	2.500
697.8325	697.8416	697.8564	697.8723	697.8892	697.9080	32.4221
0.02417	0.09828	0.02377	8.194	12.486	759.5486	3.000
702.1116	702.1211	702.1389	702.1609	702.1858	702.2151	57.3335
0.05383	0.21997	0.05267	8.502	12.725	805.4622	3.500
709.2380	709.2502	709.2761	709.3105	709.3530	709.4048	96.0574
0.09781	0.40290	0.09490	8.868	12.993	859.9858	4.000
720.7498	720.7661	720.8054	720.8608	720.9324	721.0215	138.9844
0.14397	0.59861	0.13829	9.169	13.276	904.7522	4.500
737.3613	737.3809	737.4275	737.4958	737.5864	737.6997	167.0525
0.18047	0.75619	0.17189	9.343	13.541	930.5681	5.000
755.9929	756.0134	756.0630	756.1360	756.2327	756.3533	174.2144
0.20449	0.86122	0.19369	9.423	13.761	942.5264	5.500
774.4011	774.4209	774.4690	774.5400	774.6335	774.7502	167.7761
0.21874	0.92391	0.20651	9.465	13.934	948.8191	6.000
791.5173	791.5366	791.5820	791.6484	791.7354	791.8438	156.9753
0.22670	0.95912	0.21363	9.500	14.068	953.9397	6.500
807.1509	807.1697	807.2122	807.2739	807.3545	807.4543	146.4854
0.23101	0.97827	0.21747	9.531	14.174	958.5190	7.000
821.4392	821.4568	821.4976	821.5547	821.6289	821.7200	136.7991
0.23332	0.98852	0.21951	9.547	14.256	961.0144	7.500
833.5640	833.5796	833.6135	833.6616	833.7234	833.7991	127.2153
0.23454	0.99395	0.22060	9.535	14.316	959.0920	8.000
844.1970	844.2117	844.2432	844.2871	844.3411	844.4075	114.6046
0.23518	0.99682	0.22117	9.476	14.350	950.4001	8.500
853.2158	853.2292	853.2559	853.2922	853.3367	853.3901	97.0100

9 92.031 RC=0

PARTICLE DIAMETER = 400.00 LOADING RATIO = 5.0

XA	XP	XC	VG	VP	TG	DL
T(1)	T(2)	T(3)	T(4)	T(5)	TS	DIF
0.0	0.0	0.0	7.995	8.800	730.0000	0.0
680.0000	680.0000	680.0000	680.0000	680.0000	680.0000	50.0000
0.00010	0.00041	0.00010	7.927	10.262	719.9412	0.500
684.3848	684.3945	684.4124	684.4331	684.4575	684.4846	35.4565
0.00038	0.00155	0.00038	7.874	11.305	712.0591	1.000
687.0212	687.0295	687.0432	687.0593	687.0764	687.0945	24.9646
0.00118	0.00479	0.00117	7.859	12.062	709.7644	1.500
688.8621	688.8701	688.8835	688.8975	688.9114	688.9265	20.8379
0.00343	0.01389	0.00339	7.899	12.625	715.6643	2.000
690.6008	690.6096	690.6235	690.6396	690.6563	690.6746	24.9897
0.00947	0.03843	0.00934	8.013	13.064	732.6465	2.500
692.7612	692.7703	692.7866	692.8057	692.8254	692.8479	39.7986
0.02419	0.09842	0.02379	8.230	13.434	764.9302	3.000
695.7351	695.7461	695.7686	695.7974	695.8330	695.8752	69.0549
0.05361	0.21933	0.05240	8.568	13.778	815.2957	3.500
700.5476	700.5625	700.5952	700.6414	700.6987	700.7705	114.5251
0.09695	0.40027	0.09383	8.972	14.127	875.3987	4.000
708.0854	708.1042	708.1504	708.2183	708.3079	708.4197	166.9790
0.14229	0.59398	0.13609	9.314	14.478	926.3306	4.500
718.4517	718.4749	718.5322	718.6204	718.7388	718.8877	207.4429
0.17820	0.75097	0.16866	9.527	14.809	957.9844	5.000
730.6335	730.6594	730.7239	730.8230	730.9558	731.1233	226.8611
0.20196	0.85666	0.18978	9.639	15.101	974.6284	5.500
743.3123	743.3379	743.4033	743.5044	743.6401	743.8125	230.8159
0.21616	0.92048	0.20222	9.703	15.348	984.2273	6.000
755.7063	755.7322	755.7974	755.8965	756.0300	756.1987	228.0286
0.22418	0.95677	0.20918	9.752	15.555	991.4041	6.500
767.5496	767.5742	767.6360	767.7312	767.8591	768.0208	227.3933
0.22857	0.97676	0.21297	9.789	15.728	996.9072	7.000
778.7632	778.7874	778.8474	778.9385	779.0615	779.2163	217.6909
0.23094	0.98758	0.21500	9.804	15.871	999.1736	7.500
789.3149	789.3384	789.3953	789.4819	789.5981	789.7441	209.4294
0.23221	0.99338	0.21609	9.781	15.984	995.7041	8.000
798.9890	799.0110	799.0645	799.1440	799.2490	799.3811	196.3230
0.23289	0.99647	0.21669	9.791	16.064	983.7915	8.500
807.4958	807.5159	807.5632	807.6326	807.7230	807.8381	175.9534

6 95.346 RC=0

APPENDIX G

PARAMETER ESTIMATION

The steepest descent method due to Rosenbrock was programmed in Fortran IV to solve the problem of finding the characteristic parameter vector \underline{a} of a system of differential equations of the form

$$\frac{dx}{dt} = g(\underline{x}, \underline{a}, t)$$

It was assumed that n different experiments were performed with the known initial conditions $\underline{x}_j(0)$ $j = 1, 2, \dots, n$ and that some or all of the state variables were measured at several discrete times. Given the model and the data, the parameter vector is found such that the unweighted least squares are minimized.

The Fortran IV program listed on the following pages, is broken up into a main line and five subroutines. The purpose of each subroutine is stated in the comment cards at the beginning. The main line program reads in the data and controls the stepping procedure. Comment cards in the main line program defined each variable which is read in as data. All of the subroutines are general except for the subroutine SLOPE, which defines the functions and hence must be supplied for the functional models being tested. Two models were proposed in the present study for the partial oxidation of n-butane. The models were later used to predict the temperature profiles and conversions for a number of other runs by Anderson⁽¹⁾. The runs used for this purpose were runs 11, 12, 13, 14 and 17 in his work. The experimental results for these runs are given below in Tables G-1 to G-5. The models were also used to predict the overall behaviour of the transported bed reactor.

TABLE G.1

Experimental Results for Run 11

Inlet Composition:	Oxygen 6.3519	Nitrogen 23.8951
	Butane 69.7530	Mole Per Cent
Inlet Temperature:	705°F	
Pressure:	53.50 psia	
Inlet Flow Rate:	11.46 lb/hr	

Length Along Reactor ft	Conversion <u>n</u> -Butane	Conversion Oxygen	Temperature Gas °F	Temperature Wall °F
2.54	0.0702	0.6374	851	1027
3.43			1032	
4.31	0.1670	0.9420	1009	949
5.2			988	
6.1	0.1865	0.9471	964	906
6.9			947	
7.88	0.1974	0.9486	932	883

TABLE G.2

Experimental Results for Run 12

Inlet Composition: Oxygen 6.2946 Nitrogen 23.6798
 Butane 70.0256 Mole Per Cent
 Inlet Temperature: 704°F
 Pressure: 53.50 psia
 Inlet Flow Rate: 13.58 lb/hr

Length Along Reactor ft	Conversion <u>n</u> -Butane	Conversion Oxygen	Temperature Gas °F	Temperature Wall °F
2.54	0.01712	0.2491	698	727
3.43			1023	
4.31	0.1168	0.7810	1036	975
5.2			1013	
6.1	0.1803	0.9485	989	934
6.9			973	
7.88	0.1940	0.9481	959	912

TABLE G.3

Experimental Results for Run 13

Inlet Composition: Oxygen 6.4688 Nitrogen 24.3352
 Butane 69.1960 Mole Per Cent
 Inlet Temperature: 705°F
 Pressure: 53.5 psia
 Inlet Gas Flow Rate: 12.21 lb/hr

Length Along Reactor ft	Conversion Butane	Conversion Oxygen	Temperature Gas °F	Temperature Wall °F
2.54	0.0740	0.9450	800	1076
3.43			1045	
4.31	0.1436	0.9550	1026	958
5.2			1000	
6.1	0.1919	0.9582	975	913
6.9			940	
7.88	0.2136	0.9577	940	885

TABLE G.4

Experimental Results for Run 14

Inlet Composition: Oxygen 6.4688 Nitrogen 24.3352
 Butane 69.1960 Mole Per Cent
 Inlet Temperature: 696°F
 Reactor Pressure: 53.5 psia
 Inlet Flow Rate: 12.21 lb/hr

Length Along Reactor ft	Conversion Butane	Conversion Oxygen	Temperature Gas °F	Temperature Wall °F
2.54	0.0151	0.1154	678	705
3.43			896	
4.31	0.1473	0.9082	1040	958
5.2			1015	
6.1	0.1923	0.9507	983	909
6.9			954	
7.88	0.2172	0.9497	941	878

TABLE G.5

Experimental Results for Run 17

Inlet Composition: Oxygen 7.2378 Nitrogen 27.2277
 Butane 65.5345 Mole Per Cent
 Inlet Temperature: 681°F
 Reactor Pressure: 53.5 psia
 Inlet Gas Flow Rate: 12.8 lb/hr

Length Along Reactor ft	Conversion Butane	Conversion Oxygen	Temperature Gas °F	Temperature Wall °F
2.54	0.0093	0.0302	653	637
3.43			656	
4.31	0.0259	0.2849	697	-
5.2			939	
6.1	0.1640	0.8157	1058	980
6.9			1023	
7.88	0.2068	0.9639	994	916

The computer program with some sample output is now presented.

C PARAMETER

C PARAMETER

C THE PURPOSE OF THIS PROGRAM IS TO IDENTIFY CER-
C TAIN UNKNOWN PARAMETERS IN A SYSTEM OF ORDINARY
C DIFFERENTIAL EQUATIONS. THE DIFFERENTIAL EQUA-
C TIONS REPRESENT A PHYSICAL SYSTEM FROM WHICH
C EXPERIMENTAL DATA HAS BEEN OBTAINED. ROSENBROCK'S
C METHOD OF STEEPEST DESCENT METHOD HAS BEEN USED
C TO ESTIMATE THE PARAMETERS FROM THE GIVEN DATA.
C

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COMMON ISTEP,NPITOT,LRT
COMMON A1(20),A2(20),A3(20),A4(20),A5(20),C6(20)
COMMON YO2(20),YN2(20),YC4(20),CBT(20),COX(20)
COMMON WG(20),PR(20),GG(20),NWT,NDS,TB,RR,WM,DRR
DIMENSION XO(20,8),TC(20,20),XB1(20,20,8),C1(12)
DIMENSION KS(10),KSF(10),KF(10),NC(20,20)
DIMENSION NP(20),NPIJ(20,20),NPITOT(20),KSI(20,20,8)
DIMENSION DS(10),WT(10),STM(20)
DIMENSION PRE(20,20,8)
DOUBLE PRECISION ELAM(10),OV(10,10),PAR1(10),PAR3(10)
DOUBLE PRECISION SS,VAR1,VAR3,CT,VAR2
DOUBLE PRECISION SMXMN
```

C IN ORDER TO USE THIS PROGRAM, THE DIFFERENTIAL
C EQUATION MUST BE NORMALISED SUCH THAT
C 1 THE STATE VARIABLES DO NOT DIFFER BY MORE THAN
C AN ORDER OF MAGNITUDE.
C 2 THE INDEPENDENT VARIABLES VARIES FROM ZERO TO A
C VALUE NOT EXCEEDING 10, WITH THE INITIAL CONDITION
C BEING GIVEN AT ZERO.
C 3 THE ELEMENTS OF THE PARAMETER VECTOR ARE OF THE
C SAME ORDER OF MAGNITUDE.

C THE MAIN LINE PROGRAM HAS THE FUNCTIONS OF READING
C IN THE DATA SETS, DETERMINE THE SUCCESS/FAILURE
C OF EACH STEP IN RIDGE TRACKING, DETERMINE THE STEP
C SIZE AND DECIDE ON THE ROTATION OF AXES.

C THE AUXILLIARY SUBROUTINES REQUIRED ARE

C VARIA-

C GENERATE THE SOLUTION GIVEN THE PARAMETERS.

C GENER-

C RUNGE KUTTA METHOD OF INTEGRATION TO SOLVE THE
C DIFFERENTIAL EQUATIONS.

C ROTAT-

C ROTATE THE AXES USING THE GRAM-SCHMIDT ORTHOGONA-
C LIZATION PROCESS.

C FORS-

[illegible]

IN ORDER TO USE THIS WINDOW, THE DIFFERENTIAL
EQUATION MUST BE REWRITTEN SUCH THAT
THE STATE VARIABLES DO NOT EXCEED 3000. THIS
IS DONE BY MAGNITUDE.
THE INDEPENDENT VARIABLE VARIES FROM 0 TO 1
VALUE NOT EXCEEDING 10, WITH THE INITIAL CONDITION
BEING GIVEN BY 1000.
THE ELEMENT OF THE RESPONSE VECTOR FOR THE
SAME ORDER OF MAGNITUDE.

THE MAIN LINE PROGRAM WAS THE FUNCTION OF
IN THE DATA SETS, OBTAINING THE SUCCESSIVE
OF EACH STEP IN RING TRACKING, DETERMINING THE
SIZE AND DECISION ON THE RATION OF DATA.
THE AUXILIARY SUBROUTINES-REQUIRED ARE
VARI-
DETERMINE THE SOLUTION GIVEN THE PARALLEL.
MEMBER-
LONG RATIO METHOD OF INTERPOLATION TO FIND THE
DIFFERENTIAL RATIONS.
NOTES-
ROTATE THE AXIS USING THE QUANT-20000 METHOD-
LITATION PROFS.
ENDS-

C PARAMETER ... (CONT'D)

C OBTAINS A POLYNOMIAL FOR REACTOR WALL TEMPERA-
C TURE. USUALLY THIS ROUTINE WAS USED SEPARATELY.
C SLOPE
C SUPPLIES THE FUNCTIONS.
C

SMXMN=1.D+0
READ(5,41)WMO,WN2,WC4,RR,TB,DRR
DRR=DRR/12.0
WRITE(6,41)WMO,WN2,WC4,RR,TB,DRR
41 FORMAT(6F12.5)
ARR=0.785*DRR**2

C THE FOLLOWING INTEGERS ARE READ IN ON A 16I5
C FORMAT.

C NE THE NO. OF STATE VARIABLES. NE 11

C NK THE NO. OF PARAMATERS. NK 11

C NDS THE NO. OF DATA SETS. NDS 21

C MAXR MAXIMUM NUMBER OF TRIALS

C MAXS MAXIMUM NUMBER OF STAGES

C NW NUMBER OF DATA POINTS GIVEN FOR WALL
C TEMPERATURE

C MF ORDER OF POLINOMIALS FOR WALL TEMPERATURE
C PROFILE

READ(5,1)NE,NK,NDS,MAXR,MAXS,NW,MF
WRITE(6,1)NE,NK,NDS,MAXR,MAXS,NW,MF

C PAR1 THE INITIAL GUESS FOR THE PARAMETER VECTOR IS
C READ IN ON A 5E16.6 FORMAT.

READ(5,41)(PAR1(I),I=1,NK)
WRITE(6,11)(PAR1(I),I=1,NK)

C THE FOLLOWING CONTROL VARIABLES ARE READ IN ON A

[illegible]

1981 THE INITIAL QUEST FOR THE HIGHEST QUALITY
LEAD IN THE MARKET.

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2804 JOURNAL OF CLIMATE

WAS THE WM. OF DATA SETS. WAS 1
HARR KATHIN NUMBER OF PRIS

(2.5.14) $T(M) \cong T(M)$

[illegible]

C PARAMETER ... (CONT'D)

C 4E16.6 FORMAT.

C KPN NORMALIZATION FLAG FOR PARAMETER VECTOR

C KPN=0 NORMALIZATION DESIRED

C KPN=-1 NORMALIZATION NOT DESIRED

C NWT WALL TEMPERATURE FLAG

C NWT=0 NON ADIABATIC, WALL TEMPERATURES GIVEN

C NWT=1 ADIABATIC

C READ(5,12)SS,KPN,NWT

C WRITE(6,12)SS,KPN,NWT

11 FORMAT(5E16.6)

12 FORMAT(E16.6,5X,2I5)

C NPTOT=0

C THE DATA FOR EACH EXPERIMENT ARE READ IN

C SEQUENTIALLY AS GIVEN BELOW. ALL INTEGERS ARE READ

C IN ON A 16I5 FORMAT AND ALL OTHER DATA ON A 8F10.6

C FORMAT. THE DATA IS PRINTED OUT EXACTLY AS IT IS

C READ IN.

C T IS THE INDEPENDENT VARIABLE.

C DO 101 I=1,NDS

C READ(5,1)NRUN

C WRITE(6,1)NRUN

C READ(5,18)A1(I),A2(I),A3(I),A4(I)

18 FORMAT(4F15.0)

C WRITE(6,23)A1(I),A2(I),A3(I),A4(I)

23 FORMAT(10X,4F12.6)

C READ(5,11)WG(I),PR(I),STM(I),YO2(I)

C WRITE(6,11)WG(I),PR(I),STM(I),YO2(I)

C READ(5,19)YN2(I),YC4(I)

C WRITE(6,19)YN2(I),YC4(I)

19 FORMAT(2E16.6)

C WM=YO2(I)*WMO+YN2(I)*WN2+YC4(I)*WC4

C WG(I)=WG(I)/ARR

C GG(I)=WG(I)/WM

C DG=(WM*PR(I))/(10.73*STM(I))

C CBT(I)=YC4(I)*DG/WM

C COX(I)=YO2(I)*DG/WM

(...)

...

...

...

...

...

...

...

...

...

...

C PARAMETER ... (CONT'D)

C XO(I,J) THE INTIAL CONDITION FOR THE J TH STATE
C VARIABLE FOR THE I TH EXPERIMENT.
C

```
READ(5,2) (XO(I,J),J=1,NE)
WRITE(6,2)(XO(I,J),J=1,NE)
XO(I,NE)=(XO(I,NE)+460.0)/1185.0
```

C NP(I) THE NO. OF VALUES OF T FOR WHICH DATA ARE
C GIVEN IN THE I TH EXPERIMENT.
C

```
READ(5,1) NP(I)
WRITE(6,1)NP(I)
M1=NP(I)
```

C NPIJ(I,J) THE NO. OF DATA POINTS WHICH ARE GIVEN
C FOR THE J TH VALUE OF T FOR WHICH DATA ARE
C GIVEN FOR THE I TH EXPERIMENT.
C

```
READ(5,1) (NPIJ(I,J),J=1,M1)
WRITE(6,1)(NPIJ(I,J),J=1,M1)
```

C TC(I,J) THE VALUE OF THE J TH VALUE OF T FOR WHICH
C DATA ARE GIVEN FOR THE I TH EXPERIMENT.
C

```
READ(5,2) (TC(I,J),J=1,M1)
WRITE(6,2)(TC(I,J),J=1,M1)
```

C NC(I,J) THE NO. OF INTEGRATION POINTS REQUIRED
C BETWEEN TC(I,J) AND TC(I-1,J) WITH TC(0,J)
C BEING TAKEN AS ZERO.
C

```
READ(5,1) (NC(I,J),J=1,M1)
WRITE(6,1)(NC(I,J),J=1,M1)
NPITOT(I)=0
DO 100 J=1,M1
M2=NPIJ(I,J)
NPITOT(I)=NPITOT(I)+M2
```

C KSI(I,J,K) THE STATE VARIABLE INDEX OF THE K TH
C DATA POINT AT TC(I,J).
C

```
READ(5,1) (KSI(I,J,K),K=1,M2)
WRITE(6,1)(KSI(I,J,K),K=1,M2)
```


C PARAMETER ... (CONT'D)

C XB1(I,J,K) THE VALUE OF THE K TH DATA POINT AT
C TC(I,J) WITH THE INDEX KSI(I,J,K).
C

 READ(5,2) (XB1(I,J,K),K=1,M2)
 WRITE(6,3)(XB1(I,J,K),K=1,M2)
 XB1(I,J,M2)=(XB1(I,J,M2)+460.0)/1185.0
100 CONTINUE
101 NPTOT=NPTOT+NPITOT(I)

C
C THE TOTAL NO. OF DATA POINTS IS WRITEN OUT.
C
C

 WRITE(6,22) NPTOT
22 FORMAT('OTHE TOTAL NO. OF DATA POINTS IS ',I5)
1 FORMAT(16(1X,I4))
2 FORMAT(8F10.5)
3 FORMAT(1X,8F10.5)

C
C IF THE TOTAL NO. OF DATA POINTS EXCEEDS 500 THEN
C THE PROGRAM IS TERMINATED.
C
C

 IF(NPTOT.LE.500) GOTO 120
 WRITE(6,21)
21 FORMAT('ONO. OF DATA POINTS EXCEEDS 500')
 STOP

C
C
C GENERATE INITIAL SET OF ORTHOGONAL VECTORS AND
C NULL SCALING FACTORS
C PAR3 VECTOR TO STORE THE PARAMETERS
C

120 WRITE(6,403)
403 FORMAT(1H1)
173 DO 5 I=1,NK
 KSF(I)=0
 5 PAR3(I)=PAR1(I)
14 DO 67 I=1,NK
 DO 6 J=1,NK
 6 OV(I,J)=0.0D+00
67 OV(I,I)=1.0D+00
 LRT=0
 ISTEP=0

... ..

... ..

C
C
C

... ..

C
C
C
C

... ..

... ..

C
C
C
C
C

... ..

... ..

C
C
C
C
C
C
C

... ..

... ..

C PARAMETER ... (CONT'D)

C CALCULATION OF FUNCTION VALUE FOR INITIAL GUESSES
C

CALL VARIA (NE,NK,PRE,NC,KSI,NP,NPTOT,PAR1,XB1,XO,VAR2
*,TC,NPIJ)
LRT=-1

C VAR3 VECTOR TO STORE THE VARIANCE/

VAR2=VAR2*SMXMN
VAR1=VAR2
VAR3=VAR1
WRITE(6,531)VAR3
531 FORMAT(5X,41HVARIANCE WITH INITIAL PARAMETER VALUES =
*,D18.8)

C COMMENCE ROSENBROCK ALGORITHM
C

DO 7 KKK=1,MAXS
WRITE(6,303)KKK
303 FORMAT(10X,11HBEGIN STAGE,I3)

C GENERATE INITIAL STEPSIZES AND SUCCESS/FAILURE
C FLAGS
C

DO 85 I=1,NK
ELAM(I)=SS*(10.D+00)**KSF(I)
KS(I)=1
85 KF(I)=1

C COMMENCE RIDGE TRACKING
C

DO 80 KLP=1,MAXR
IF(KLP.EQ.MAXR)GOTO579
ISTEP=ISTEP+1
DO 90 II=1,NK

C ADJUSTMENT OF PARAMETERS
C

93 DO 9 I=1,NK
9 PAR1(I)=PAR1(I)+OV(II,I)*ELAM(II)

C CALCULATE NEW FUNCTION VALUE AND COMPARE TO OLD
C ONE
C

C PARAMETER ... (CONT'D)

CALL VARIA (NE,NK,PRE,NC,KSI,NP,NPTOT,PAR1,XB1,XO,VAR2
*,TC,NPIJ)

VAR2=VAR2*SMXMN

IF(LRT.EQ.0) GO TO 95

GO TO 94

95 WRITE(6,535) VAR2

535 FORMAT(9X,11HVARIANCE = ,D18.5)

94 LRT=-1

IF(VAR1-VAR2) 10,203,203

C SUCCESSFUL STEP, ADJUST STEPSIZE AND SET SUCCESS
C FLAG
C

203 VAR1=VAR2
ELAM(II)=ELAM(II)*3.0D+00
IF(KS(II))89,81,89
89 KS(II)=0
GO TO 81

C UNSUCCESSFUL STEP, RETURN TO PREVIOUS PARAMETER
C VALUES, ADJUST STEPSIZE AND DIRECTION AND SET
C FAILURE FLAG
C

10 DO 13 I=1,NK
PAR1(I)=PAR1(I)-ELAM(II)*OV(II,I)
13 CONTINUE
ELAM(II)=ELAM(II)/(-2.0D+00)
IF(KS(II))81,91,81
91 KS(II)=-1

C TEST FOR OSCILLATORY STEPPING STATUS AND MAGNITUDE
C OF STEPSIZE
C

81 DO 82 I=1,NK
505 IF(KS(I))82,90,90
82 CONTINUE
GO TO 83
90 CONTINUE
80 CONTINUE
83 CONTINUE

ISTEP=0

C ROTATION OF AXES
C

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1--(11)24 19

$$D_0 = 10 \cdot \ln((71)28) = 11$$
$$(100010101, 5-1) \setminus (11) \text{ 用 } 113 = (11) \text{ 用 } 113$$

3 CONTINUED

$$(I_1, I_2) \in \mathcal{P}(I_1, I_2) \text{ if } (I_1, I_2) = (I_1, I_2) \text{ or } (I_1, I_2) = (I_1, I_2)$$

2014, 1=1 2 3 4 5 6 7 8 9 10 11 12

WOLFSON

10 07 72

 $\sigma = (11)23 \quad \text{or}$

9. 10. 22 ((11)2X)+1

$$f(\mathbf{v}_1, \mathbf{v}_2) = \begin{pmatrix} 1 & 1 \end{pmatrix} A \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \end{pmatrix} A \begin{pmatrix} 1 \\ 1 \end{pmatrix} =$$
$$E_{AB}V' = I_{AB}V \quad 509$$

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$$205, 205, 111 \quad (5.820 - 1.820) \div 11$$
$$I = T \cdot I_{\text{A2}}$$
$$f(x) = \frac{1}{2} \left(1 + \frac{x}{\sqrt{1+x^2}} \right)$$

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C PARAMETER ... (CONT'D)

```

CALL ROTAN(NK,PAR1,PAR3,OV)

      DO 40 I=1,NK
      PAR1(I)=PAR1(I)/((10.D+00)**KSF(I))
40  CONTINUE
      DO 17 I=1,NK
      PAR1(I)=PAR1(I)*((10.D+00)**KSF(I))
17  PAR3(I)=PAR1(I)
      WRITE(6,591)KKK,(PAR1(I),I=1,NK)
591  FORMAT(1X,31HPARAMETER VALUES AFTER ROTATION,I4,2X
*,3HARE//10X,3F10
2.2)
      IF(DABS(VAR1-VAR3)-1.D-08) 30,30,310
310  VAR3=VAR1
      IF(KPN)301,30,301
301  LRT=0
      7  CONTINUE
      WRITE(6,401)KKK
401  FORMAT(1H,5X,33HTHE SYSTEM DID NOT CONVERGE AFTER,I4
*,1X,6HSTAGES)
      STOP
      30  IF(KPN-1) 102,209,102
102  KPN=1
      CALL TORM(NK,PAR1,KSF)
      DO 33 I=1,NK
      33  PAR3(I)=PAR1(I)
      GO TO 14
209  DO 31 I=1,NK
      31  PAR1(I)=PAR1(I)/((10.D+00)**KSF(I))
      WRITE(6,597)(PAR1(I),I=1,NK)
597  FORMAT(1H,5X,30HTHE FINAL PARAMETER VALUES ARE//20X
*,7F8.2)
300  CONTINUE
579  WRITE(6,581)KLP
581  FORMAT(10X,33HTHE SYSTEM DID NOT CONVERGE AFTER,I4,2X
*,6HTRIALS)
      STOP
      END

```


SUBROUTINE VARIA

```

SUBROUTINE VARIA(NE,NK,PRE,NC,KSI,NP,NPTOT,CO,XB1,XO
*,VAR2,TC,NPIJ)
COMMON ISTEP,NPITOT,LRT
COMMON A1(20),A2(20),A3(20),A4(20),A5(20),C6(20)
COMMON Y02(20),YN2(20),YC4(20),CBT(20),COX(20)
COMMON WG(20),PR(20),GG(20),NWT,NDS,TB,RR,WM,DRR
DOUBLE PRECISION CO,VAR2,SUMA,SUMB,CF
DIMENSION CO(10),X(20,8),XBAR(20,20,8),XB1(20,20,8)
DIMENSION NC(20,20),KSI(20,20,8),NP(40),XO(20,8),TC(20
*,20)
DIMENSION NPIJ(20,20),NPITOT(20)
DIMENSION PRE(20,20,8)

C
C      GENERATE THE SOLUTION FROM THE APPROXIMATE
C      PARAMETERS.
C
C
95  FORMAT(5X,9HFOR TRIAL,I3,2X,8HDATA SET,I3,2X,4HWITH,I4
*,2X,6HPOINTS
2/5X,24HTHE INITIAL CONDITION IS/)
96  FORMAT(10X,8F10.4)
97  FORMAT(5X,17HTHE CONSTANTS ARE/10X,9E12.4/)
SUMB=0.0
DO 103 I=1,NDS
INR=I
IF(LRT)71,72,71
72  WRITE(6,95)ISTEP,I,NPITOT(I)
XO(I,NE)=XO(I,NE)*1185.0-460.0
WRITE(6,96)(XO(I,II),II=1,NE)
XO(I,NE)=XO(I,NE)/1185.0+460.0/1185.0
WRITE(6,97)(CO(II),II=1,NK)
71  T=0.0
DO 104 II=1,NE
104  X(1,II)=XO(I,II)
M1=NP(I)
DO 103 J=1,M1
NCJ=NC(I,J)
F=NCJ
H=(TC(I,J)-T)/F
CALL GENER(NE,NK,NCJ,H,T,X,CO,INR)
M2=NPIJ(I,J)
DO 105 K=1,M2
S=KSI(I,J,K)
XBAR(I,J,K)=X(1,S)

C      SUMA=ABS(XB1(I,J,K)-XBAR(I,J,K))*PRE(I,J,K)

SUMA=ABS(XB1(I,J,K)-XBAR(I,J,K))

```


SUBROUTINE VARIA ... (CONT'D)

```
SUMB=SUMB+SUMA**2
105 CONTINUE
103 CONTINUE
NPS=NK+1
CF=FLOAT(NPTOT-NPS)
VAR2=SUMB/CF
RETURN
END
```


SUBROUTINE GENER

SUBROUTINE GENER(NE,NK,NCJ,H,T,X,PAR1,INR)

```

C
C      THE PURPOSE OF THIS SUBROUTINE IS TO GENERATE THE
C      SOLUTION OF THE SYSTEM OF DIFFERENTIAL EQUATIONS
C      GIVEN A SET OF PARAMETERS. THE 4 TH ORDER RUNGE
C      KUTTA PROCEEDURE IS USED.
C
C
COMMON ISTEP,NPITOT,LRT
COMMON A1(20),A2(20),A3(20),A4(20),A5(20),C6(20)
COMMON YD2(20),YN2(20),YC4(20),CBT(20),COX(20)
COMMON WG(20),PR(20),GG(20),NWT,NDS,TB,RR,WM,DRR
REAL KP
DOUBLE PRECISION PAR1
DIMENSION X(20,8),XA(20,8),PAR1(10),KP(4,10),G(10)
*,NPITOT(20)

C
      DO 300 N=1,NCJ
      DO 101 II=1,4
      GOTO(102,103,104,105),II
102  TA=T
      DO 106 I=1,NE
106  XA(1,I)=X(1,I)
      GOTO 107
103  TA=T+0.5*H
      DO 108 I=1,NE
108  XA(1,I)=X(1,I)+0.5*KP(1,I)
      GOTO 107
104  DO 109 I=1,NE
109  XA(1,I)=X(1,I)+0.5*KP(2,I)
      GOTO 107
105  TA=T+H
      DO 110 I=1,NE
110  XA(1,I)=X(1,I)+KP(3,I)
107  CALL SLOPE(NE,NK,XA,G,PAR1,II,TA,INR)
      DO 101 I=1,NE
101  KP(II,I)=H*G(I)
      T=TA
      DO 100 I=1,NE
100  X(1,I)=X(1,I)+(KP(1,I)+2.0*(KP(2,I)+KP(3,I))+KP(4,I))
      */6.0
300  CONTINUE
      IF(LRT)71,72,71
72  X(1,NE)=X(1,NE)*1185.0-460.0
      WRITE(6,500)T,(X(1,I),I=1,NE)
      X(1,NE)=X(1,NE)/1185.0+460.0/1185.0

```

APPENDIX A

THE FOLLOWING TABLES GIVE THE VALUES OF THE FUNCTIONS

THE FUNCTIONS $f(x)$ AND $g(x)$ ARE DEFINED BY THE FOLLOWING TABLES. THE VALUES OF $f(x)$ AND $g(x)$ ARE GIVEN FOR x IN THE RANGE $0 \leq x \leq 1$.

TABLE A.1

x	$f(x)$	$g(x)$
0.0	0.0000	0.0000
0.1	0.0995	0.0995
0.2	0.1960	0.1960
0.3	0.2895	0.2895
0.4	0.3795	0.3795
0.5	0.4655	0.4655
0.6	0.5470	0.5470
0.7	0.6245	0.6245
0.8	0.6975	0.6975
0.9	0.7655	0.7655
1.0	0.8280	0.8280

TABLE A.2

x	$f(x)$	$g(x)$
0.0	0.0000	0.0000
0.1	0.0995	0.0995
0.2	0.1960	0.1960
0.3	0.2895	0.2895
0.4	0.3795	0.3795
0.5	0.4655	0.4655
0.6	0.5470	0.5470
0.7	0.6245	0.6245
0.8	0.6975	0.6975
0.9	0.7655	0.7655
1.0	0.8280	0.8280

SUBROUTINE GENER ... (CONT'D)

```
500 FORMAT(7X,1H*,10F10.4)
```

```
71 RETURN
```

```
END
```


SUBROUTINE ROTAN

SUBROUTINE ROTAN(P,PAR1,PAR3,OV)

C THIS SUBROUTINE ROTATES THE AXES USING THE GRAM
C SCHMIDT ORTHOGONALIZATION PROCESS.
C

```
COMMON ISTEP,NPITOT,LRT
COMMON A1(20),A2(20),A3(20),A4(20),A5(20),C6(20)
COMMON YO2(20),YN2(20),YC4(20),CBT(20),COX(20)
COMMON WG(20),PR(20),GG(20),NWT,NDS,TB,RR,WM,DRR
DIMENSION NPITOT(20)
INTEGER P
DOUBLE PRECISION S,SO,DOG
DOUBLE PRECISION A(10,10),B(10,10),PAR1(10),PAR3(10)
*,OV(10,10)
```

C

```
DO 1 I=1,P
DO 1 J=1,P
A(I,J)=0.0D+00
1 B(I,J)=0.0D+00
DO 2 I=1,P
DO 2 J=1,P
A(I,J)=PAR1(J)-PAR3(J)
2 B(I,J)=A(I,J)
SO=0.0D+00
DO 3 J=1,P
3 SO=SO+A(1,J)**2
S=SO**0.5
DO 4 J=1,P
4 OV(1,J)=A(1,J)/S
DO 5 I=2,P
MI=I-1
DO 6 K=1,MI
DOG=0.0D+00
DO 7 J=1,P
7 DOG=DOG+OV(K,J)*A(K,J)
DO 8 J=1,P
8 B(I,J)=B(I,J)-DOG*OV(K,J)
6 CONTINUE
SO=0.0D+00
DO 9 J=1,P
9 SO=SO+B(I,J)**2
S=SO**0.5
DO 10 J=1,P
10 OV(I,J)=B(I,J)/S
5 CONTINUE
RETURN
END
```

```
*.OV(10,10)
DOUBLE PRECISION A(10,10), B(10,10), C(10,10), D(10,10)
DOUBLE PRECISION S(10,10), T(10,10), U(10,10), V(10,10)
INTEGER P
```

[illegible]

SUBROUTINE TORM

SUBROUTINE TORM (P,PAR1,KSF)

C THIS SUBROUTINE MAPS THE PARAMETERS BETWEEN 0.1
C AND 1.0
C

```
COMMON ISTEP,NPITOT,LRT
COMMON A1(20),A2(20),A3(20),A4(20),A5(20),C6(20)
COMMON Y02(20),YN2(20),YC4(20),CBT(20),COX(20)
COMMON WG(20),PR(20),GG(20),NWT,NDS,TB,RR,WM,DRR
INTEGER P
DOUBLE PRECISION PAR1(10),PP1
DIMENSION KSF(10)
DIMENSION NPITOT(20)
```

C

```
DO 1 I=1,P
1 KSF(I)=0
DO 2 I=1,P
PP1=DLOG10(PAR1(I))
IF(PP1) 3,4,4
3 KSF(I)=PP1-1
GO TO 2
4 KSF(I)=PP1
2 CONTINUE
RETURN
END
```


SUBROUTINE FORS

SUBROUTINE FORS(X,Y,N,NN,M,C1)

C FORSYTHE POLYNOMIAL CURVE FIT USING LEAST SQUARE CRITERIA

C

C

C THE VECTOR C1 CONTAINS THE COEFFICIENTS OF THE POWER
C SERIES EXPANSION OF THE FORSYTHE POLYNOMIAL FIT.C $Y=C1(1)+C1(2)*X+C1(3)*X*X+...$ C THERE ARE M+1 COEFFICIENTS WHERE M IS THE ORDER OF
C THE FIT

C

INTEGER N,I,J,M

INTEGER L,LL

REAL P(10,20),X(20),Y(20),F(20),DIFF(20),W(20)
*,PERER(20)

REAL A(10),B(10),C(10),S,V,Q,T,STDEV

REAL D(10,10),C1(10),Z(20)

C X DISTANCE ALONG REACTOR FT

C Y TEMPERATURE IN DEGREES RANKINE

C N NUMBER OF DATA POINTS

C M ORDER OF POLYNOMIAL

C THE LENGTH AND TEMPERATURE IN THIS PROGRAM ARE
C NORMALIZED.

C

DO 10 I=1,N

F(I)=0.0

W(I)=1.0

P(1,I)=1.0

X(I)=X(I)/10.0

Y(I)=(Y(I)+460.0)/1185.0

10 CONTINUE

B(1)=0.0

DO 11 J=1,M

IF(J-1)12,12,31

31 T=0.0

DO 13 I=1,N

T=T+W(I)*X(I)*P(J-1,I)*P(J,I)

13 CONTINUE

B(J)=T/V

12 V=0.0

S=0.0

Q=0.0

DO 14 I=1,N

V=V+W(I)*P(J,I)**2

S=S+W(I)*X(I)*P(J,I)**2

Q=Q+W(I)*Y(I)*P(J,I)

14 CONTINUE

SUBROUTINE FORS ... (CONT'D)

```

A(J+1)=S/V
C(J)=Q/V
DO 15 I=1,N
  IF(J-1)16,16,32
32 P(J+1,I)=(X(I)-A(J+1))*P(J,I)-B(J)*P(J-1,I)
  GOTO 15
16 P(J+1,I)=(X(I)-A(J+1))*P(J,I)
15 CONTINUE
  STDEV=0.0
  DO 17 I=1,N
    F(I)=F(I)+C(J)*P(J,I)
    DIFF(I)=ABS(Y(I)-F(I))
    PERER(I)=100.0*DIFF(I)/Y(I)
    STDEV=STDEV+DIFF(I)**2
17 CONTINUE
  STDEV=STDEV/FLOAT(N-1)
  STDEV=SQRT(STDEV)
  IF(J-M)11,33,11
33 WRITE(6,3) J,STDEV
  WRITE(6,4)
  WRITE(6,5) (I,A(I),B(I-1),I=2,J)
  WRITE(6,6)
  WRITE(6,7) (C(I),I=1,J)
  WRITE(6,8)
  WRITE(6,9) (I,X(I),Y(I),F(I),DIFF(I),PERER(I),I=1,N)
11 CONTINUE

```

C EXPANSION OF FORSYTHE POLYNOMIAL

C

```

L=M+1
DO 19 I=1,L
DO 19 J=1,L
  D(I,J)=0.0
  IF(I-J)19,35,19
35 D(I,J)=1.0
19 CONTINUE
  D(1,1)=0.0
  D(2,3)=-A(2)
  D(2,4)=A(2)*A(3)-B(2)
  D(3,4)=-(A(2)+A(3))
  D(2,5)=-A(2)*A(3)*A(4)+B(2)*A(4)+A(2)*B(3)
  D(3,5)=A(2)*A(3)+A(4)*A(2)+A(3)*A(4)-B(2)-B(3)
  D(4,5)=-(A(2)+A(3)+A(4))
  DO 20 J=6,L
    LL=J-1
    DO 20 I=2,LL
      D(I,J)=D(I-1,J-1)-A(J-1)*D(I,J-1)-B(J-2)*D(I,J-2)
20 CONTINUE
  DO 22 J=1,M

```


SUBROUTINE FORS ... (CONT'D)

```

S=0.0
DO 21 I=1,M
S=S+C(I)*D(J+1,I+1)
21 CONTINUE
C1(J)=S
22 CONTINUE
WRITE(6,40)
WRITE(6,7)(C1(I),I=1,M)
DO 341 I=1,N
Z(I)=C1(1)+C1(2)*X(I)+C1(3)*X(I)**2+C1(4)*X(I)**3
*+C1(5)*X(I)**4
Z(I)=Z(I)*1185.0-460.0
341 CONTINUE
WRITE(6,373)(X(I),Y(I),Z(I),I=1,N)
373 FORMAT(10X,3E18.6)
1 FORMAT(I5)
2 FORMAT(2E16.8)
3 FORMAT(16H1AN EXPANSION OF,I4,2X,59HFORSYTHE
* ORTHOGONAL POLYNOMIAL
31S HAS A STANDARD DEVIATION OF,E17.8)
4 FORMAT(30HJT THE FORSYTHE COEFFICIENTS ARE/38HJ J
* A(J)
1 B(J-1)//)
5 FORMAT(1X,I2,2X,2E17.8)
6 FORMAT(35HJT THE COEFFICIENTS C(1).....C(J) ARE)
7 FORMAT(3X,6E17.8)
8 FORMAT(6HK I,7X,4HX(I),13X,4HY(I),13X,4HF(I),11X
*,7HDIFF(I),6X,
1 13HPERCENT ERROR//)
9 FORMAT(1X,I4,5E17.8)
40 FORMAT(32HJT THE POLYNOMIAL COEFFICIENTS ARE)
RETURN
END

```


SUBROUTINE SLOPE

```
SUBROUTINE SLOPE(NE,NK,X,G,PAR1,II,TA,INR)
```

C
C
C
C

```
THIS SUBROUTINE CALCULATES THE VALUE OF THE  
FUNCTIONS
```

```
COMMON ISTEP,NPITOT,LRT
COMMON A1(20),A2(20),A3(20),A4(20),A5(20),C6(20)
COMMON Y02(20),YN2(20),YC4(20),CBT(20),COX(20)
COMMON WG(20),PR(20),GG(20),NWT,NDS,TB,RR,WM,DRR
DIMENSION X(20,8),G(10),PAR1(10),NPITOT(20)
DOUBLE PRECISION PAR1
XA=X(1,1)
XB=X(1,2)
XC=X(1,3)
TG=X(1,4)
A6=34.47
A7=-.01998
A8=34.07
A9=10.0
A10=34.68
E1=PAR1(1)
E2=-5.211
E3=PAR1(2)
E4=-9.66
E5=PAR1(3)
Q1=1.0E-04
R1=1.0
S1=0.0001
T1=1.0
U1=1.0E-04
HR1=-75.0*1000.0
HR2=60.0*1000.0
HR3=70.0*1000.0
HR4=-60.0*1000.0
HR5=40.9*1000.0
HR6=-15.5*1000.0
HR7=-40.0*1000.0
HF=2.8
CAO=CBT(INR)
CBO=COX(INR)
WQ=WG(INR)
GM=GG(INR)
31 TQ=TG*TB
14 TD=TA/10.0
TW=A1(INR)+A2(INR)*TD+A3(INR)*TD**2+A4(INR)*TD**3
12 DG=(WM*PR(INR))/(10.73*TQ)
CPG=0.1903+1.8E-04*TQ-3.147E-08*TQ**2
UG=0.04598+0.00004556*(TQ-660.0)
```


SUBROUTINE SLOPE ... (CONT'D)

```

      TKG=0.01762+0.0000233*(TQ-660.0)
      HW=0.027*(WQ*CPG)**.78*(TKG/DRR)**.22
      HW=HW*HF
      B2=DG/WQ
      F3=CPG*WM*GM
      F3=1.0/F3
      F3=F3/TB
16  F1=(4.0*HW)/(DRR*CPG*WQ)
36  EA=Q1*(EXP(A6-E1*RR/TG))
      EB=R1*(EXP(A7-E2*RR/TG))
      EC=S1*(EXP(A8-E3*RR/TG))
      ED=T1*(EXP(A9-E4*RR/TG))
      EE=U1*(EXP(A10-E5*RR/TG))
      C1=EA*(1.0-XA)*(1.0-XB)
      C3=EC*(1.0-XB)*XC
      C7=ED*(1.0-XA)
      C8=EE*CAO*(1.0-XA)
      C10=C1*CAO*CBO
      C11=C3*CAO*CBO
      EQ=1.0/EB
      DER1=C10+C7*CAO*(2.0*C10+C11)
      DER2=DER1+C10+C11
      DER3=DER1/(1.0+EB)-C11
      DER1=DER1+EE*CAO*(1.0-XA)
      PP=HR1*C10+HR4*C11+HR7*C8+(C10/(1.0+EQ))*(HR2+EQ*HR3)
      *+(2.0*C10+C11
      2)*((C7*CAO/(1.0+EQ))*(HR2+EQ*HR3)+HR5*C7*CAO+HR6)
      PP=PP*F3
      G(4)=PP-F1*(TG-TW)
      G(1)=DER1/CAO*B2
      G(2)=DER2/CBO*B2
      G(3)=DER3/CAO*B2
      RETURN
      END

```


\$RUN -LOAD#

08:52.03

32.00000	28.00000	58.00000	0.42470	1185.00000
----------	----------	----------	---------	------------

4	3	3	20	20	10	4
---	---	---	----	----	----	---

0.480000D 02	0.280000D 02	0.480000D 02
--------------	--------------	--------------

0.100000D-01	1	0
--------------	---	---

62

0.980907	-0.783087	3.145142	-2.562305
----------	-----------	----------	-----------

0.122000E 02	0.537000E 02	0.115500E 04	0.741259E-01
--------------	--------------	--------------	--------------

0.278856F 00	0.647018E 00
--------------	--------------

0.0	0.0	0.0	695.00000
-----	-----	-----	-----------

5

3	1	3	1	3
---	---	---	---	---

2.54000	3.43000	4.31000	5.20000	6.10000
---------	---------	---------	---------	---------

40	20	20	20	20
----	----	----	----	----

1	2	4
---	---	---

0.01600	0.16000	672.00000
---------	---------	-----------

4

676.00000

1	2	4
---	---	---

0.03300	0.24600	705.00000
---------	---------	-----------

4

913.00000

1	2	4
---	---	---

0.12800	0.88800	970.00000
---------	---------	-----------

63

0.976492	-0.714916	3.815235	-3.453047
----------	-----------	----------	-----------

0.126000E 02	0.536000E 02	0.116200E 04	0.854260E-01
--------------	--------------	--------------	--------------

0.321362E 00	0.593213E 00
--------------	--------------

0.0	0.0	0.0	702.00000
-----	-----	-----	-----------

5

3	1	3	1	3
---	---	---	---	---

2.54000	3.43000	4.31000	5.20000	6.10000
---------	---------	---------	---------	---------

10	10	10	20	20
----	----	----	----	----

1	2	4
---	---	---

0.00750	0.09220	684.00000
---------	---------	-----------

4

696.00000

1	2	4
---	---	---

0.07190	0.38670	820.00000
---------	---------	-----------

4

1041.00000

1	2	4
---	---	---

0.19190	0.946701	032.00000
---------	----------	-----------

64

0.982055	-0.943544	3.766500	-3.126618
----------	-----------	----------	-----------

0.107000E 02	0.535800E 02	0.115200E 04	0.798990E-01
--------------	--------------	--------------	--------------

0.300572E 00	0.619529E 00
--------------	--------------

0.0	0.0	0.0	692.00000
-----	-----	-----	-----------

5

3	1	3	1	3
---	---	---	---	---

2.54000	3.43000	4.31000	5.20000	6.10000
---------	---------	---------	---------	---------

10	10	10	20	20
----	----	----	----	----

1	2	4
---	---	---

0.00340	0.11500	666.00000
---------	---------	-----------

4

670.00000

1	2	4
---	---	---

0.03740	0.21200	714.00000
---------	---------	-----------

4

G-27

825.00000

1

2

4

0.14800

0.935001 025.00000

THE TOTAL NO. OF DATA POINTS IS 33

FOR TRIAL 0 DATA SET 1 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0 0.0 0.0 694.9998
THE CONSTANTS ARE

	0.48000 02	0.28000 02	0.48000 02		
*	2.5400	0.1420	0.9479	0.0120	825.8323
*	3.4300	0.1575	0.9935	0.0126	744.0569
*	4.3100	0.1629	0.9987	0.0126	731.9275
*	5.2000	0.1684	0.9997	0.0127	754.0413
*	6.1000	0.1768	1.0000	0.0127	783.7324

FOR TRIAL 0 DATA SET 2 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0 0.0 0.0 701.9998
THE CONSTANTS ARE

	0.48000 02	0.28000 02	0.48000 02		
*	2.5400	0.1954	0.9738	0.0163	867.2234
*	3.4300	0.2152	0.9979	0.0167	788.3411
*	4.3100	0.2251	0.9997	0.0167	793.9182
*	5.2000	0.2389	1.0000	0.0167	829.2295
*	6.1000	0.2610	1.0000	0.0167	861.2881

FOR TRIAL 0 DATA SET 3 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0 0.0 0.0 691.9998
THE CONSTANTS ARE

	0.48000 02	0.28000 02	0.48000 02		
*	2.5400	0.1749	0.9859	0.0144	789.8713
*	3.4300	0.1832	0.9981	0.0145	718.8108
*	4.3100	0.1874	0.9996	0.0145	721.2251
*	5.2000	0.1929	0.9999	0.0145	753.5271
*	6.1000	0.2026	1.0000	0.0145	788.2585

VARIANCE WITH INITIAL PARAMETER VALUES = 0.141206640 00
BEGIN STAGE 1

PARAMETER VALUES AFTER ROTATION 1 ARE

51.64 29.21 47.39

BEGIN STAGE 2

FOR TRIAL 1 DATA SET 1 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0 0.0 0.0 694.9995
THE CONSTANTS ARE

	0.51650 02	0.29210 02	0.47390 02		
*	2.5400	0.0155	0.0670	0.0007	661.3490
*	3.4300	0.0247	0.1246	0.0013	687.8939
*	4.3100	0.0449	0.2539	0.0028	748.6179
*	5.2000	0.1060	0.6039	0.0074	863.2603
*	6.1000	0.1986	0.9361	0.0122	877.5842

FOR TRIAL 1 DATA SET 2 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0 0.0 0.0 701.9995
THE CONSTANTS ARE

	0.51650 02	0.29210 02	0.47390 02		
*	2.5400	0.0186	0.0670	0.0009	690.2244
*	3.4300	0.0366	0.1553	0.0022	748.4155
*	4.3100	0.1071	0.4828	0.0077	892.6655

* 5.2000 0.2775 0.9499 0.0168 937.4548
 * 6.1000 0.3396 0.9942 0.0176 888.9609
 FOR TRIAL 1 DATA SET 3 WITH 11 POINTS
 THE INITIAL CONDITION IS

0.0 0.0 0.0 691.9995

THE CONSTANTS ARE

0.5165D 02 0.2921D 02 0.4739D 02
 * 2.5400 0.0177 0.0744 0.0009 653.1692
 * 3.4300 0.0293 0.1437 0.0017 685.7280
 * 4.3100 0.0588 0.3196 0.0040 766.5051
 * 5.2000 0.1594 0.7933 0.0113 902.9426
 * 6.1000 0.2413 0.9786 0.0143 855.9133

VARIANCE = 0.48362D-02

PARAMETER VALUES AFTER ROTATION 2 ARE

52.05 29.34 47.33

BEGIN STAGE 3

FOR TRIAL 1 DATA SET 1 WITH 11 POINTS
 THE INITIAL CONDITION IS

0.0 0.0 0.0 694.9993

THE CONSTANTS ARE

0.5206D 02 0.2934D 02 0.4733D 02
 * 2.5400 0.0138 0.0514 0.0005 657.9277
 * 3.4300 0.0209 0.0927 0.0010 681.2859
 * 4.3100 0.0358 0.1818 0.0020 732.9546
 * 5.2000 0.0795 0.4336 0.0051 830.2747
 * 6.1000 0.1843 0.8686 0.0114 900.5774

FOR TRIAL 1 DATA SET 2 WITH 11 POINTS
 THE INITIAL CONDITION IS

0.0 0.0 0.0 701.9993

THE CONSTANTS ARE

0.5206D 02 0.2934D 02 0.4733D 02
 * 2.5400 0.0163 0.0510 0.0007 686.0559
 * 3.4300 0.0301 0.1130 0.0016 737.0479
 * 4.3100 0.0778 0.3301 0.0051 849.9036
 * 5.2000 0.2579 0.8917 0.0159 966.2771
 * 6.1000 0.3461 0.9886 0.0178 900.2563

FOR TRIAL 1 DATA SET 3 WITH 11 POINTS
 THE INITIAL CONDITION IS

0.0 0.0 0.0 691.9993

THE CONSTANTS ARE

0.5206D 02 0.2934D 02 0.4733D 02
 * 2.5400 0.0154 0.0562 0.0006 648.9614
 * 3.4300 0.0241 0.1046 0.0012 677.0015
 * 4.3100 0.0446 0.2216 0.0027 742.7549
 * 5.2000 0.1203 0.6042 0.0084 880.6299
 * 6.1000 0.2397 0.9554 0.0142 881.4865

VARIANCE = 0.37058D-02

PARAMETER VALUES AFTER ROTATION 3 ARE

51.95 29.35 47.34

BEGIN STAGE 4

FOR TRIAL 1 DATA SET 1 WITH 11 POINTS
 THE INITIAL CONDITION IS

0.0 0.0 0.0 694.9990

THE CONSTANTS ARE

	0.5194D 02	0.2935D 02	0.4734D 02		
*	2.5400	0.0141	0.0542	0.0006	658.4771
*	3.4300	0.0216	0.0977	0.0010	682.1990
*	4.3100	0.0371	0.1915	0.0021	734.8035
*	5.2000	0.0826	0.4539	0.0054	833.9961
*	6.1000	0.1861	0.8776	0.0115	897.6887

FOR TRIAL 1 DATA SET 2 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0	0.0	0.0	701.9990
-----	-----	-----	----------

THE CONSTANTS ARE

	0.5194D 02	0.2935D 02	0.4734D 02		
*	2.5400	0.0167	0.0538	0.0007	686.7078
*	3.4300	0.0310	0.1191	0.0016	738.5239
*	4.3100	0.0812	0.3480	0.0054	854.5527
*	5.2000	0.2605	0.8998	0.0160	962.5815
*	6.1000	0.3450	0.9891	0.0177	858.7952

FOR TRIAL 1 DATA SET 3 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0	0.0	0.0	691.9990
-----	-----	-----	----------

THE CONSTANTS ARE

	0.5194D 02	0.2935D 02	0.4734D 02		
*	2.5400	0.0158	0.0593	0.0007	649.5994
*	3.4300	0.0249	0.1103	0.0013	678.1211
*	4.3100	0.0464	0.2335	0.0028	745.3091
*	5.2000	0.1248	0.6277	0.0087	884.0779
*	6.1000	0.2397	0.9580	0.0142	878.2036

VARIANCE = 0.36441D-02

PARAMETER VALUES AFTER ROTATION 4 ARE

51.81	29.36	47.34
-------	-------	-------

BEGIN STAGE 5

FOR TRIAL 1 DATA SET 1 WITH 11 POINTS

THE INITIAL CONDITION IS

0.0	0.0	0.0	694.9988
-----	-----	-----	----------

THE CONSTANTS ARE

	0.5180D 02	0.2936D 02	0.4734D 02		
*	2.5400	0.0145	0.0575	0.0006	659.1204
*	3.4300	0.0223	0.1035	0.0011	683.2505
*	4.3100	0.0385	0.2025	0.0022	736.8784
*	5.2000	0.0859	0.4758	0.0057	837.7932
*	6.1000	0.1877	0.8859	0.0116	894.4363

FOR TRIAL 1 DATA SET 2 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0	0.0	0.0	701.9988
-----	-----	-----	----------

THE CONSTANTS ARE

	0.5180D 02	0.2936D 02	0.4734D 02		
*	2.5400	0.0172	0.0571	0.0008	687.4697
*	3.4300	0.0322	0.1263	0.0017	740.2156
*	4.3100	0.0850	0.3680	0.0057	859.6157
*	5.2000	0.2628	0.9072	0.0161	958.5291
*	6.1000	0.3437	0.9896	0.0177	897.3318

FOR TRIAL 1 DATA SET 3 WITH 11 POINTS
THE INITIAL CONDITION IS

0.0	0.0	0.0	691.9988
-----	-----	-----	----------

THE CONSTANTS ARE

	0.5180D 02	0.2936D 02	0.4734D 02		
*	2.5400	0.0163	0.0629	0.0007	650.3433
*	3.4300	0.0258	0.1169	0.0014	679.4031
*	4.3100	0.0484	0.2470	0.0030	748.1467
*	5.2000	0.1295	0.6517	0.0091	886.9753
*	6.1000	0.2394	0.9603	0.0142	874.8674
VARIANCE =		0.36231D-02			

B30020